

# Scattering in $\mathcal{PT}$ -Symmetric Quantum Mechanics

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## Abstract

A general formalism is worked out for the description of one-dimensional scattering in non-hermitian quantum mechanics and constraints on transmission and reflection coefficients are derived in the cases of  $\mathcal{P}$ ,  $\mathcal{T}$  or  $\mathcal{PT}$  invariance of the Hamiltonian. Applications to some solvable  $\mathcal{PT}$ -symmetric potentials are shown in detail.

Our main original results concern the association of reflectionless potentials with asymptotic exact  $\mathcal{PT}$  symmetry and the peculiarities of separable kernels of non-local potentials in connection with Hermiticity,  $\mathcal{T}$  invariance and  $\mathcal{PT}$  invariance.

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# 1 Introduction

Since the seminal paper by Bender and Boettcher [1], research on  $\mathcal{PT}$ -symmetric quantum mechanics has been mainly focused on bound states, either with real energies, or in complex conjugate energy pairs, while relatively few authors have studied scattering states of Hamiltonians with both discrete and continuous spectra [2, 3, 4, 5].

This gap has been recently bridged, at least in part, by a review paper on complex absorbing potentials [6], covering the more extended topics of one-dimensional scattering in non-hermitian quantum mechanics, with some general formulae valid for complex  $\mathcal{PT}$ -symmetric potentials. Nonetheless, we think it worthwhile to go into further details in the latter case, while paying the due credit to the authors of Ref. [6], and apply our formalism to some examples of solvable potentials for the sake of clarity.

In any case, we share the philosophy of ref. [6], i. e. to consider  $\mathcal{PT}$ -symmetric potentials as complex potentials defined on the real axis. Therefore, when we define complex coordinate shifts, we mean this as a method of generating complex potentials depending on a real coordinate.

The main purpose of the present paper is thus to give a general description of one-dimensional scattering in non-hermitian quantum mechanics with the Hamiltonian,  $H$ , invariant either under parity,  $\mathcal{P}$ , or time reversal,  $\mathcal{T}$ , or their product,  $\mathcal{PT}$ , in the case  $H$  is not separately invariant under  $\mathcal{P}$  and  $\mathcal{T}$ . We do not intend, however, to provide here physical motivations for  $\mathcal{PT}$  symmetry, nor to elaborate on the significance of violation of hermiticity and unitarity in quantum mechanics. The reader interested in these topics can consult a wide list of references, in particular the recent works [7, 8, 9] and references therein.

In the present work, we limit ourselves to a framework in which the scattering potentials vanish asymptotically: in particular, we exclude potentials diverging at infinity, like those considered in Ref.[10]. Therefore, our asymptotic wave functions are linear superpositions of plane waves and the present approach closely resembles standard scattering theory described in text-books on quantum mechanics, such as Ref.[11], in the limit in which Hermiticity and  $\mathcal{P}$ – and  $\mathcal{T}$ –symmetries hold.

What we try to achieve is to assemble a comprehensive and self-contained formalism for discussing scattering problems in one-dimensional quantum mechanics. With this formalism available, we provide suitable examples, which should make the reader capable of elaborating his/her judgement on the relevance of the subject of  $\mathcal{PT}$  symmetry, including some contributions to a better understanding of “exact”  $\mathcal{PT}$  symmetry. Due to the relation of the Schrödinger equation to the classical Helmholtz equation, our formalism may be accommodated to deal with optics [6, 12] with refraction index characterized by “handedness” [13].

In addition, we try to clarify the interplay between  $\mathcal{T}$  invariance and hermiticity, displaying a complex non-local solvable potential in which hermiticity does not force  $\mathcal{T}$  invariance, but can be compatible with  $\mathcal{PT}$  invariance. To our

knowledge, a  $\mathcal{PT}$ -symmetric non-local potential is introduced and worked out here for the first time.

We hope that our work is sufficiently self-contained, such as not to require any particular specific background of the reader. The paper definitely has topical review aspects, though it does not pretend to give a complete list of references. There are, however, relevant original results, in particular for non-local separable potentials.

The paper is organized as follows: section 2 describes the basic formalism of one-dimensional scattering in non-hermitian quantum mechanics, section 3 introduces symmetries under which  $H$  may be invariant, section 4 defines density currents and continuity equations, section 5 applies the formalism worked out in the previous three sections to some solvable potentials. Finally, section 6 is devoted to conclusions.

## 2 $L$ - $R$ Representation

We start from the general time-dependent Schrödinger equation

$$-\frac{\partial^2}{\partial x^2}\psi(x,t) + \int K(x,y)\psi(y,t)dy = i\frac{\partial}{\partial t}\psi(x,t), \quad (1)$$

written in units  $\hbar = 2m = 1$ . For a monochromatic wave, of energy  $\omega$ , the time dependence of the wave function is

$$\psi(x,t) = \Psi(x)e^{-i\omega t}. \quad (2)$$

In the present work, unless otherwise stated, we consider local potentials, for which the kernel  $K$  reduces to

$$K(x,y) = \delta(x-y)V(y) \quad (3)$$

If eqs.(2-3) hold, eq. (1) reduces to the time independent Schrödinger equation satisfied by  $\Psi(x)$

$$H\Psi \equiv \left(-\frac{d^2}{dx^2} + V(x)\right)\Psi = k^2\Psi, \quad (4)$$

with  $k = \sqrt{\omega}$  ( $> 0$ ) the wave number. In order to solve eq.(4), it is convenient to work in a two dimensional Hilbert space where the basis vectors are the kets  $|R\rangle$  and  $|L\rangle$  (and the corresponding bras  $\langle R|$  and  $\langle L|$ ). In configuration space, with the choice of the time dependent phase given by eq. (2),

$$\langle x|R, k \rangle \sim e^{ikx} \quad (5)$$

represents a plane wave travelling from left to right and

$$\langle x|L, k \rangle \sim e^{-ikx} \quad (6)$$

a wave travelling from right to left. In the following, the explicit  $k$  dependence of the basis vectors will be omitted, whenever not strictly necessary, for simplicity of notation.

In coordinate space, the asymptotic states, i.e., outside the (finite) range of the potential, can be expressed at  $x \rightarrow -\infty$  as

$$|\Psi_{x \rightarrow -\infty}\rangle = A_-|R\rangle + B_-|L\rangle \quad (7)$$

and, at  $x \rightarrow +\infty$ , as

$$|\Psi_{x \rightarrow +\infty}\rangle = A_+|R\rangle + B_+|L\rangle, \quad (8)$$

or, in terms of wave functions

$$\Psi(x) = \begin{cases} A_-e^{ikx} + B_-e^{-ikx} & x \rightarrow -\infty \\ A_+e^{ikx} + B_+e^{-ikx} & x \rightarrow +\infty \end{cases} \quad (9)$$

In the case of a finite-range local potential, Eq. (4) admits a general solution written as a linear combination of two independent solutions,  $F_1(x)$  and  $F_2(x)$ , with non-zero Wronskian, whose asymptotic expressions are both of the form:

$$\lim_{x \rightarrow \pm\infty} F_m(x) = a_{m\pm}e^{ikx} + b_{m\pm}e^{-ikx}, \quad (m = 1, 2) \quad (10)$$

The  $a_{m\pm}$  and  $b_{m\pm}$  are simply related to the asymptotic amplitudes  $A_{\pm}$  and  $B_{\pm}$

$$\begin{aligned} A_{\pm} &= \alpha a_{1\pm} + \beta a_{2\pm} \\ B_{\pm} &= \alpha b_{1\pm} + \beta b_{2\pm}. \end{aligned} \quad (11)$$

If  $\Psi_1(x) = \alpha F_1(x) + \beta F_2(x)$ , inserted into Eq. (2), gives rise to a wave moving from  $x = -\infty$  to  $x = +\infty$ , the amplitude of the regressive wave vanishes at  $+\infty$ :

$$B_+ = 0 \implies \frac{\beta}{\alpha} = -\frac{b_{1+}}{b_{2+}},$$

and the transmission and reflection coefficients of the wave moving from left to right are immediately written as

$$\begin{aligned} T_{L \rightarrow R} \equiv \frac{A_+}{A_-} &= \frac{\alpha a_{1+} + \beta a_{2+}}{\alpha a_{1-} + \beta a_{2-}} \\ &= \frac{a_{2+}b_{1+} - a_{1+}b_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}}. \end{aligned}$$

$$\begin{aligned} R_{L \rightarrow R} \equiv \frac{B_-}{A_-} &= \frac{\alpha b_{1-} + \beta b_{2-}}{\alpha a_{1-} + \beta a_{2-}} \\ &= \frac{b_{1+}b_{2-} - b_{1-}b_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}}. \end{aligned}$$

The asymptotic form of  $\Psi_1(x)$  is thus, neglecting a global normalization factor

$$\begin{aligned}\Psi_1(x) &\sim e^{ikx} + R_{L \rightarrow R} e^{-ikx}, \quad x \rightarrow -\infty \\ &\sim T_{L \rightarrow R} e^{ikx}, \quad x \rightarrow +\infty.\end{aligned}\tag{12}$$

Similarly, if  $\Psi_2(x)$  gives rise to a wave moving from  $x = +\infty$  to  $x = -\infty$ , the amplitude of the progressive wave vanishes at  $-\infty$ :

$$\tilde{A}_- = 0 \implies \frac{\beta}{\alpha} = -\frac{a_{1-}}{a_{2-}},$$

and the transmission and reflection coefficients of the wave moving from right to left are:

$$\begin{aligned}T_{R \rightarrow L} &\equiv \frac{\tilde{B}_-}{\tilde{B}_+} = \frac{\alpha b_{1-} + \beta b_{2-}}{\alpha b_{1+} + \beta b_{2+}} \\ &= \frac{a_{2-} b_{1-} - a_{1-} b_{2-}}{a_{2-} b_{1+} - a_{1-} b_{2+}}.\end{aligned}$$

$$\begin{aligned}R_{R \rightarrow L} &\equiv \frac{\tilde{A}_+}{\tilde{B}_+} = \frac{\alpha a_{1+} + \beta a_{2+}}{\alpha b_{1+} + \beta b_{2+}} \\ &= \frac{a_{1+} a_{2-} - a_{1-} a_{2+}}{a_{2-} b_{1+} - a_{1-} b_{2+}}.\end{aligned}$$

As a consequence, the asymptotic form of  $\Psi_2(x)$  is

$$\begin{aligned}\Psi_2(x) &\sim T_{R \rightarrow L} e^{-ikx}, \quad x \rightarrow -\infty \\ &\sim e^{-ikx} + R_{R \rightarrow L} e^{ikx}, \quad x \rightarrow +\infty\end{aligned}\tag{13}$$

When we compute the Wronskian of  $\Psi_1$  and  $\Psi_2$ , defined as

$$W(x) = \Psi_1(x) \frac{d}{dx} \Psi_2(x) - \Psi_2(x) \frac{d}{dx} \Psi_1(x),$$

we readily obtain  $W(-\infty) = -2ikT_{R \rightarrow L}$  and  $W(+\infty) = -2ikT_{L \rightarrow R}$ . Therefore, a necessary condition for the Wronskian to be constant on the  $x$  axis is  $T_{L \rightarrow R} = T_{R \rightarrow L}$ . It is easy to check that  $dW/dx = 0$  for any well-behaved local potential. Therefore, the equality of the two transmission coefficients is satisfied for any such potential.

The scattering matrix,  $S$ , connects the outgoing states at  $t \rightarrow +\infty$  to the ingoing ones at  $t \rightarrow -\infty$

$$|\Psi_{out}\rangle = S |\Psi_{in}\rangle.\tag{14}$$

The  $S$  matrix elements are directly linked to the transmission and reflection coefficients. In this basis,  $|R\rangle$  and  $|L\rangle$  can be rewritten as

$$|R\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$|L\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

If we have an ingoing wave of  $|R\rangle$  type, then the outgoing wave is

$$\begin{pmatrix} A_+ \\ B_- \end{pmatrix} = S \begin{pmatrix} A_- \\ 0 \end{pmatrix} \implies \begin{pmatrix} T_{L \rightarrow R} \\ R_{L \rightarrow R} \end{pmatrix} = S \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

If the ingoing wave is of  $|L\rangle$  type, we obtain, with the same procedure

$$\begin{pmatrix} R_{R \rightarrow L} \\ T_{R \rightarrow L} \end{pmatrix} = S \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (15)$$

As a consequence of the above equations, the  $S$  matrix elements are explicitly given by

$$S = \begin{pmatrix} S_{RR} & S_{RL} \\ S_{LR} & S_{LL} \end{pmatrix} = \begin{pmatrix} T_{L \rightarrow R} & R_{R \rightarrow L} \\ R_{L \rightarrow R} & T_{R \rightarrow L} \end{pmatrix}. \quad (16)$$

Note that our  $T_{i \rightarrow j}(R_{i \rightarrow j})$  corresponds to  $T^i(R^i)$  of Ref. [6] and to  $t_j(r_j)$  of Ref. [5]. Our definition of  $S$  matrix is the same as that of Refs. [6, 5], while in the  $S$  matrix defined in the book by Merzbacher [11] the rows are exchanged with respect to ours. The latter author introduces also the transfer matrix,  $M$ , yielding the asymptotic states at  $x \rightarrow -\infty$  when applied to those at  $x \rightarrow +\infty$  (see Ref.[11], formula (6.24)). In our basis,  $M$ , like  $S$ , is a  $2 \times 2$  matrix, whose elements are easily expressed in terms of right and left transmission and reflection coefficients.

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = M \begin{pmatrix} A_+ \\ B_+ \end{pmatrix}. \quad (17)$$

If the incident wave is of  $|R\rangle$  type, the effect of  $M$  is expressed by the equation

$$\begin{pmatrix} 1 \\ R_{L \rightarrow R} \end{pmatrix} = M \begin{pmatrix} T_{L \rightarrow R} \\ 0 \end{pmatrix},$$

while, if the incident wave is of  $|L\rangle$  type, the following equation holds

$$\begin{pmatrix} 0 \\ T_{R \rightarrow L} \end{pmatrix} = M \begin{pmatrix} R_{R \rightarrow L} \\ 1 \end{pmatrix}.$$

From the equations given above, we obtain

$$\begin{pmatrix} M_{RR} & M_{RL} \\ M_{LR} & M_{LL} \end{pmatrix} = \begin{pmatrix} 1/T_{L \rightarrow R} & -R_{R \rightarrow L}/T_{L \rightarrow R} \\ R_{L \rightarrow R}/T_{L \rightarrow R} & T_{R \rightarrow L} - R_{R \rightarrow L}R_{L \rightarrow R}/T_{L \rightarrow R} \end{pmatrix}, \quad (18)$$

with  $\det M = T_{R \rightarrow L}/T_{L \rightarrow R}$ .

In general, any matrix,  $O$ , in the  $R - L$  basis

$$O \equiv \begin{pmatrix} O_{RR} & O_{RL} \\ O_{LR} & O_{LL} \end{pmatrix} \quad (19)$$

can be written also as a linear combination of basic dyadic operators

$$\Omega_{ij} = |i\rangle\langle j|, \quad j = R, L \quad (20)$$

in the form

$$O = O_{RR}\Omega_{RR} + O_{RL}\Omega_{RL} + O_{LR}\Omega_{LR} + O_{LL}\Omega_{LL} \quad (21)$$

This notation will be used in the following sections in the discussion of the invariance of the Hamiltonian with respect to various transformations.

### 3 $\mathcal{P}$ , $\mathcal{T}$ and $\mathcal{PT}$ Symmetries

In the present section, we study the transformation properties of the Hamiltonian with respect to  $\mathcal{P}$ ,  $\mathcal{T}$  and  $\mathcal{PT}$  reflections. With particular reference to  $\mathcal{PT}$  transformations, it is useful to introduce a discussion of the behaviour of vectors and matrices in the  $R - L$  basis under coordinate shifts.

#### 3.1 Coordinate Shifts

In connection with the coordinate shift  $x \rightarrow x + X_0$ , with  $X_0$  a real number,

let us define a displacement operator,  $\mathcal{D}(X_0)$ , through its action on the basis vectors  $|R\rangle$  and  $|L\rangle$

$$\begin{aligned} \mathcal{D}(X_0) |R\rangle &= e^{ikX_0} |R\rangle ; \\ \mathcal{D}(X_0) |L\rangle &= e^{-ikX_0} |L\rangle ; \end{aligned}$$

and on their dual vectors

$$\begin{aligned} \langle R| \mathcal{D}^{-1}(X_0) &= e^{-ikX_0} \langle R| ; \\ \langle L| \mathcal{D}^{-1}(X_0) &= e^{ikX_0} \langle L| . \end{aligned}$$

In matrix form

$$\mathcal{D}(X_0) = \begin{pmatrix} e^{ikX_0} & 0 \\ 0 & e^{-ikX_0} \end{pmatrix}. \quad (22)$$

Since  $X_0$  is real,  $\mathcal{D}^{-1}(X_0) = \mathcal{D}^*(X_0)$ .

The basic dyadic operators are thus transformed under  $D$  according to the obvious relations

$$\begin{aligned} \mathcal{D}(X_0) |R\rangle \langle R| \mathcal{D}^{-1}(X_0) &= |R\rangle \langle R| ; \\ \mathcal{D}(X_0) |L\rangle \langle L| \mathcal{D}^{-1}(X_0) &= |L\rangle \langle L| ; \\ \mathcal{D}(X_0) |R\rangle \langle L| \mathcal{D}^{-1}(X_0) &= e^{2ikX_0} |R\rangle \langle L| ; \\ \mathcal{D}(X_0) |L\rangle \langle R| \mathcal{D}^{-1}(X_0) &= e^{-2ikX_0} |L\rangle \langle R| . \end{aligned}$$

and a generic one-body operator, conveniently written in the form of a  $2 \times 2$  matrix, is consequently transformed as follows

$$\mathcal{D}(X_0)O\mathcal{D}^{-1}(X_0) = \mathcal{D}(X_0) \begin{pmatrix} O_{RR} & O_{RL} \\ O_{LR} & O_{LL} \end{pmatrix} \mathcal{D}^{-1}(X_0) = \begin{pmatrix} O_{RR} & e^{2ikX_0}O_{RL} \\ e^{-2ikX_0}O_{LR} & O_{LL} \end{pmatrix}. \quad (23)$$

### 3.2 Parity

We shall consider now the parity transformation

$$x \rightarrow -x, \quad p_x \rightarrow -p_x.$$

Under parity, the kets  $|R\rangle$  and  $|L\rangle$  are transformed according to

$$\begin{aligned} \mathcal{P}|R\rangle &= |L\rangle; \\ \mathcal{P}|L\rangle &= |R\rangle, \end{aligned}$$

and the bras  $\langle R|$  and  $\langle L|$  are changed as follows

$$\begin{aligned} \langle R|\mathcal{P}^{-1} &= \langle L|; \\ \langle L|\mathcal{P}^{-1} &= \langle R|. \end{aligned}$$

Hence, the four basic operators  $\Omega_{ij}$  transformed according to  $\mathcal{P}\Omega_{ij}\mathcal{P}^{-1}$  yield

$$\begin{pmatrix} \Omega_{RR} & \Omega_{RL} \\ \Omega_{LR} & \Omega_{LL} \end{pmatrix} \rightarrow \begin{pmatrix} \Omega_{LL} & \Omega_{LR} \\ \Omega_{RL} & \Omega_{RR} \end{pmatrix}. \quad (24)$$

In this basis, the parity operator can be represented by the matrix  $\mathcal{P}$  (with  $\mathcal{P}^2 = 1$ ) [5], which, acting on the left, exchanges lines, while acting on the right exchanges columns

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathcal{P}^{-1} \quad (25)$$

The Hamiltonian can be expressed as

$$H \equiv H_{RR}\Omega_{RR} + H_{RL}\Omega_{RL} + H_{LR}\Omega_{LR} + H_{LL}\Omega_{LL}, \quad (26)$$

or, in matrix form

$$H = \begin{pmatrix} H_{RR} & H_{RL} \\ H_{LR} & H_{LL} \end{pmatrix}.$$

The transformed Hamiltonian is then

$$\begin{aligned} H_P &= \mathcal{P}H\mathcal{P}^{-1} \\ &= H_{RR}\Omega_{LL} + H_{RL}\Omega_{LR} + H_{LR}\Omega_{RL} + H_{LL}\Omega_{RR} \\ &= \begin{pmatrix} H_{LL} & H_{LR} \\ H_{RL} & H_{RR} \end{pmatrix}. \end{aligned}$$



Parity invariance for the Hamiltonian,  $H_{\mathcal{P}} = H$ , therefore requires

$$H_{RR} = H_{LL} \quad (27)$$

$$H_{RL} = H_{LR}. \quad (28)$$

In the interaction picture, the  $S$  matrix is known to be the following limit of the transition operator,  $\tilde{T}(t - t_0)$  (see Ref.[11], formulae (14.49) and (20.7) )

$$S = \lim_{t \rightarrow \infty, t_0 \rightarrow -\infty} \tilde{T}(t - t_0) = \lim_{t \rightarrow \infty, t_0 \rightarrow -\infty} U_0(t) T(t - t_0) U_0^{-1}(t_0) \quad (29)$$

with

$$U_0(t) = e^{iH_0 t}, \quad H_0 = p^2 = -\frac{d^2}{dx^2} \quad (30)$$

and

$$T(t - t_0) = e^{-iH(t-t_0)} = \sum_{n=0}^{\infty} (-i)^n H^n (t - t_0)^n / n! \quad (31)$$

It is now possible to investigate the transformation of  $S$  under parity  $\mathcal{P}$ . In order to compute

$$S_{\mathcal{P}} = \mathcal{P} S \mathcal{P}^{-1} \quad (32)$$

we need

$$\begin{aligned} \mathcal{P} T(t - t_0) \mathcal{P}^{-1} &= \sum_{n=0}^{\infty} (-i)^n \mathcal{P} H^n \mathcal{P}^{-1} (t - t_0)^n / n! \\ &= \sum_{n=0}^{\infty} (-i)^n H_{\mathcal{P}}^n (t - t_0)^n / n! \\ &= \sum_{n=0}^{\infty} (-i)^n H^n (t - t_0)^n / n! = T(t - t_0), \end{aligned}$$

and  $\mathcal{P} U_0(t) \mathcal{P}^{-1} = U_0(t)$ , so that

$$S_{\mathcal{P}} = S. \quad (33)$$

Hence, the  $S$  matrix commutes with  $\mathcal{P}$ .

Therefore, if the Hamiltonian is invariant under parity, so is the  $S$  matrix, which yields, upon using eq. (16)

$$S_{RR} = S_{LL} \rightarrow T_{L \rightarrow R} = T_{R \rightarrow L} \quad (34)$$

and

$$S_{RL} = S_{LR} \rightarrow R_{R \rightarrow L} = R_{L \rightarrow R} \quad (35)$$

The last two equations are strictly analogous to those, eqs.(27) and (28), expressing the parity invariance of the Hamiltonian, and are already given in Ref. [6].

### 3.3 Generalized Parity

We shall consider the following generalized parity transformation

$$x \rightarrow X_0 - x \quad X_0 \in \mathbf{R}$$

corresponding to the reflection around the point  $X_0/2$  on the real  $x$  axis. This kind of transformation will be useful in the study of properties of potentials not centred on the origin, and can be readily expressed as the (non commutative) product of the parity operator  $\mathcal{P}$  and the coordinate shift operator  $\mathcal{D}(X_0)$

$$\mathcal{P}_G(X_0) \equiv \mathcal{P}\mathcal{D}(X_0). \quad (36)$$

Under generalized parity, the kets  $|R\rangle$  and  $|L\rangle$  are transformed as follows

$$\begin{aligned} \mathcal{P}_G(X_0)|R\rangle &= e^{ikX_0}|L\rangle \\ \mathcal{P}_G(X_0)|L\rangle &= e^{-ikX_0}|R\rangle \end{aligned}$$

and, correspondingly, the bras  $\langle R|$  and  $\langle L|$  give

$$\begin{aligned} \langle R|\mathcal{P}_G^{-1}(X_0) &= \langle L|e^{-ikX_0} \\ \langle L|\mathcal{P}_G^{-1}(X_0) &= \langle R|e^{ikX_0} \end{aligned}$$

Since the matrix  $\mathcal{P}_G(X_0)$  associated to this transformation reads in the  $|R\rangle, |L\rangle$  basis

$$\mathcal{P}_G(X_0) = \begin{pmatrix} 0 & e^{-ikX_0} \\ e^{ikX_0} & 0 \end{pmatrix}$$

and, consequently,

$$\mathcal{P}_G(X_0) = \mathcal{P}_G^{-1}(X_0),$$

the four basic operators  $\Omega_{ij}$  transformed under  $\mathcal{P}_G(X_0)\Omega_{ij}\mathcal{P}_G^{-1}(X_0)$  yield

$$\begin{pmatrix} \Omega_{RR} & \Omega_{RL} \\ \Omega_{LR} & \Omega_{LL} \end{pmatrix} \rightarrow \begin{pmatrix} \Omega_{LL} & \Omega_{LR}e^{2ikX_0} \\ \Omega_{RL}e^{-2ikX_0} & \Omega_{RR} \end{pmatrix} \quad (37)$$

Thus, the transformed Hamiltonian reads

$$\begin{aligned} H_{\mathcal{P}_G} &= \mathcal{P}_G(X_0)H\mathcal{P}_G^{-1}(X_0) \\ &= H_{RR}\Omega_{LL} + H_{RL}\Omega_{LR}e^{2ikX_0} + H_{LR}\Omega_{RL}e^{-2ikX_0} + H_{LL}\Omega_{RR} \end{aligned}$$

Invariance of the Hamiltonian under generalized parity,  $H_{\mathcal{P}_G} = H$ , is equivalent to

$$H_{RR} = H_{LL} \quad (38)$$

$$H_{RL} = H_{LR}e^{-2ikX_0}. \quad (39)$$

The behaviour of the  $S$  matrix under  $\mathcal{P}_G$  immediately follows from the  $\mathcal{P}_G$  invariance of  $H$

$$S_{\mathcal{P}} = \mathcal{P}_G(X_0)S\mathcal{P}_G^{-1}(X_0)$$

We have

$$S_{\mathcal{P}_G} = S,$$

or

$$\mathcal{P}_G(X_0)S = S\mathcal{P}_G(X_0).$$

$\mathcal{P}_G$  invariance of the  $S$  matrix corresponds to

$$S_{RR} = S_{LL} \rightarrow T_{R \rightarrow L} = T_{L \rightarrow L}$$

and

$$S_{RL}e^{ikX_0} = S_{LR}e^{-ikX_0} \rightarrow R_{R \rightarrow L}e^{ikX_0} = R_{L \rightarrow R}e^{-ikX_0}.$$

### 3.4 Time Reversal

For this case we follow the same steps as in subsection 3.2. First, we consider the consequence of the invariance property for the Hamiltonian (26), having in mind that the time reversal operator  $\mathcal{T}$  is an antiunitary operator ( $\mathcal{T} = \mathcal{T}^{-1} = \mathcal{T}^\dagger$ ). Under time reversal

$$x \rightarrow x, \quad p_x \rightarrow -p_x \quad i \rightarrow -i$$

any ket in the  $|R\rangle, |L\rangle$  basis is transformed according to

$$\mathcal{T}(\alpha|R\rangle + \beta|L\rangle) = \alpha^*|L\rangle + \beta^*|R\rangle,$$

while a bra fulfills the relation

$$(\gamma\langle R| + \delta\langle L|)\mathcal{T}^{-1} = \gamma^*\langle L| + \delta^*\langle R|$$

It is worth stressing that  $\mathcal{T}$ -invariance as such does not force the potential to be real, and hence, the Hamiltonian to be hermitian.

The  $\Omega_{ij}$  operators are now transformed into  $\mathcal{T}\Omega_{ij}\mathcal{T}^{-1}$

$$\begin{pmatrix} \Omega_{RR} & \Omega_{RL} \\ \Omega_{LR} & \Omega_{LL} \end{pmatrix} \rightarrow \begin{pmatrix} \Omega_{LL} & \Omega_{LR} \\ \Omega_{RL} & \Omega_{RR} \end{pmatrix} \quad (40)$$

which may be compared to eqs.(24) and (36). The  $\mathcal{T}$ -transformed Hamiltonian,  $H_{\mathcal{T}} = \mathcal{T}\mathcal{H}\mathcal{T}^{-1}$ , reads

$$H_{\mathcal{T}} = H_{RR}^*\Omega_{LL} + H_{RL}^*\Omega_{LR} + H_{LR}^*\Omega_{RL} + H_{LL}^*\Omega_{RR} = \begin{pmatrix} H_{LL}^* & H_{LR}^* \\ H_{RL}^* & H_{RR}^* \end{pmatrix}. \quad (41)$$

From the properties of the parity operator (25), it is easy to realize that  $H_{\mathcal{T}}$  defined in the previous equation is such that

$$\mathcal{P}H_{\mathcal{T}} = H^*\mathcal{P}, \quad (42)$$

or

$$H_{\mathcal{T}} = \mathcal{P}H^*\mathcal{P}, \quad (43)$$

where  $\mathcal{P}$  is the parity operator (25).

We now proceed to examine how the  $S$  matrix transforms under  $\mathcal{T}$  without imposing any symmetry to the Hamiltonian. Starting from the transition operator,  $\tilde{T}(t - t_0)$ , of formula (29), and using eq. (43), we have

$$\begin{aligned}
\tilde{T}_{\mathcal{T}}(t - t_0) &\equiv \mathcal{T}\tilde{T}(t - t_0)\mathcal{T}^{-1} \\
&= \mathcal{T}e^{iH_0t}\mathcal{T}^{-1} \sum_{n=0}^{\infty} \mathcal{T}(-i)^n H^n \mathcal{T}^{-1} (t - t_0)^n / n! \mathcal{T}e^{-iH_0t_0}\mathcal{T}^{-1} \\
&= e^{-iH_0t} \sum_{n=0}^{\infty} i^n H_{\mathcal{T}}^n (t - t_0)^n / n! e^{iH_0t_0} \\
&= e^{-iH_0t} \sum_{n=0}^{\infty} i^n (\mathcal{P}H^*\mathcal{P})^n (t - t_0)^n / n! e^{iH_0t_0} = \mathcal{P}\tilde{T}^*(t - t_0)\mathcal{P},
\end{aligned}$$

which, when  $t \rightarrow +\infty$  and  $t_0 \rightarrow -\infty$ , yields

$$S_{\mathcal{T}} \equiv \mathcal{T}S\mathcal{T}^{-1} = \mathcal{P}S^*\mathcal{P} = \begin{pmatrix} S_{LL}^* & S_{LR}^* \\ S_{RL}^* & S_{RR}^* \end{pmatrix}. \quad (44)$$

### 3.4.1 $H_{\mathcal{T}} = H$

For a  $\mathcal{T}$ -invariant Hamiltonian ( $H_{\mathcal{T}} = H$ ), the diagonal matrix elements are complex conjugate of each other as are the two non-diagonal ones, so that a time reversal invariant Hamiltonian is, in that basis, of the form

$$H = H_{\mathcal{T}} = \begin{pmatrix} H_{RR} & H_{RL} \\ H_{RL}^* & H_{RR}^* \end{pmatrix}. \quad (45)$$

Hence, as is well-known, this is not equivalent to hermiticity of the Hamiltonian.

Coming now to the transition operator,  $T$ , we easily obtain, under time reversal invariance of  $H$ , with the same procedure as in the previous subsection,

$$T_{\mathcal{T}}(t - t_0) = T^{-1}(t - t_0).$$

Hence,  $H = H_{\mathcal{T}}$  leads to

$$S_{\mathcal{T}} = S^{-1} \equiv \frac{1}{\det S} \begin{pmatrix} S_{LL} & -S_{RL} \\ -S_{LR} & S_{RR} \end{pmatrix}, \quad (46)$$

Simultaneous validity of Eqs. (44, 46) thus leads to the following explicit relations for the S-matrix elements :

$$\begin{aligned}
S_{RL} + S_{LR}^* \det S &= 0 \\
S_{LR} + S_{RL}^* \det S &= 0 \\
S_{LL} &= S_{LL}^* \det S \\
S_{RR} &= S_{RR}^* \det S.
\end{aligned}$$

Hence, on the assumption that all the  $S$ -matrix elements are different from zero, we obtain

$$\det S = \frac{S_{LL}}{S_{LL}^*} = \frac{S_{RR}}{S_{RR}^*} = -\frac{S_{RL}}{S_{LR}^*} = -\frac{S_{LR}}{S_{RL}^*},$$

with

$$|\det S| = 1$$

and

$$|S_{LR}| = |S_{RL}|$$

or, equivalently

$$|R_{L \rightarrow R}| = |R_{R \rightarrow L}|.$$

This also forces  $S_{LL}S_{RR}^*$ , *i.e.*  $T_{R \rightarrow L}T_{L \rightarrow R}^*$  to be real and

$$\begin{aligned} T_{L \rightarrow R}T_{R \rightarrow L}^* + |R_{L \rightarrow R}|^2 &= 1, \\ T_{R \rightarrow L}T_{L \rightarrow R}^* + |R_{L \rightarrow R}|^2 &= 1. \end{aligned}$$

### 3.4.2 $H_{\mathcal{T}} = H^\dagger$

Since, by definition,

$$H^\dagger = \begin{pmatrix} H_{RR}^* & H_{LR}^* \\ H_{RL}^* & H_{LL}^* \end{pmatrix},$$

using the explicit representation of  $H_{\mathcal{T}}$ , formula (41), we may write

$$H_{\mathcal{T}} = H^\dagger + \begin{pmatrix} H_{LL}^* - H_{RR}^* & 0 \\ 0 & H_{RR}^* - H_{LL}^* \end{pmatrix}, \quad (47)$$

which displays transparently the connection between the time reversal transformed Hamiltonian and the hermitian conjugate of the same Hamiltonian. They coincide if the diagonal matrix elements  $H_{LL}$  and  $H_{RR}$  are identical. In that case the hermiticity of the Hamiltonian forces time reversal invariance. This is what happens for a local potential, yielding the current conservation relation (see section 4). For a non-local potential, in general,  $H_{\mathcal{T}} \neq H^\dagger$ .

If we now assume, instead of time reversal invariance ( $H_{\mathcal{T}} = H$ ), the condition  $H_{\mathcal{T}} = H^\dagger$ , equivalent to the intertwining relation

$$H_{\mathcal{T}}\mathcal{T} = \mathcal{T}H = H^\dagger\mathcal{T}. \quad (48)$$

it is almost immediate to check that

$$S_{\mathcal{T}} \equiv \mathcal{T}S\mathcal{T}^{-1} = S^\dagger, \quad (49)$$

or, in explicit form

$$\begin{pmatrix} S_{LL}^* & S_{LR}^* \\ S_{RL}^* & S_{RR}^* \end{pmatrix} = \begin{pmatrix} S_{RR}^* & S_{LR}^* \\ S_{RL}^* & S_{LL}^* \end{pmatrix},$$

leading to the equality of the diagonal matrix elements

$$S_{RR} = S_{LL} \rightarrow T_{L \rightarrow R} = T_{R \rightarrow L}.$$

### 3.4.3 $H_{\mathcal{T}} = H^{\dagger} = H$

At this stage, we want to point out that if we assume, in addition to  $H = H_{\mathcal{T}}$ , also hermiticity of the Hamiltonian, i.e.,  $H = H^{\dagger}$ , we see from eq.(47) that we must have

$$H_{RR} = H_{RR}^* = H_{LL}^* = H_{LL}.$$

Thus, the diagonal matrix elements of  $H$  are equal and real.

While condition (48) may be met by Hamiltonians that are neither hermitian, nor  $\mathcal{T}$ -invariant, for instance those containing local potentials, it is met a fortiori by Hamiltonians that are both hermitian and  $\mathcal{T}$ -invariant. In the latter case, we simultaneously have  $H_{\mathcal{T}} = H \implies S_{\mathcal{T}} = S^{-1}$ , according to Eq. (46), and  $H_{\mathcal{T}} = H^{\dagger} \implies S_{\mathcal{T}} = S^{\dagger}$ , on the basis of Eq. (49). From these conditions the unitarity of the  $S$  matrix follows

$$S^{\dagger} = S^{-1}. \quad (50)$$

In terms of  $S$ -matrix elements,

$$\begin{aligned} S_{RL} + S_{LR}^* \det S &= 0 \\ S_{LR} + S_{RL}^* \det S &= 0 \\ S_{LL} &= S_{RR}^* \det S \\ S_{RR} &= S_{LL}^* \det S \end{aligned}$$

Summing up,  $\mathcal{T}$ -invariance and hermiticity of the Hamiltonian lead to

$$S^t \mathcal{P} = \mathcal{P} S \quad \text{and} \quad S^{\dagger} = S^{-1} \quad (51)$$

or, explicitly,

$$\det S = -\frac{S_{RL}}{S_{LR}^*} = -\frac{S_{LR}}{S_{RL}^*} \quad \text{and} \quad S_{LL} = S_{RR} \quad (52)$$

so that

$$|S_{LR}| = |S_{RL}| \quad \text{and} \quad |\det S| = 1 \quad (53)$$

In terms of transmission and reflection coefficients, we then have

$$\begin{aligned} T_{L \rightarrow R} &= T_{R \rightarrow L}, \\ |R_{L \rightarrow R}| &= |R_{R \rightarrow L}|. \end{aligned}$$

It is worth pointing out that our definition of  $\mathcal{T}$  is consistent with that of ref. [6], while ref. [5] adopts the following

$$\mathcal{T}' \equiv OK, \quad (54)$$

where  $K$  is the complex conjugation operator, and  $O$  is a unitary operator.

### 3.5 $\mathcal{PT}$ Symmetry

We may now try to understand the consequences of  $\mathcal{PT}$ -invariance (but not separately parity or time reversal invariance).

Any ket in the  $|R\rangle, |L\rangle$  basis is transformed under  $\mathcal{PT}$  according to

$$\mathcal{PT}(\rho|R\rangle + \sigma|L\rangle) = \rho^*|R\rangle + \sigma^*|L\rangle \quad (55)$$

while, correspondingly, for a bra

$$(\rho\langle R| + \sigma\langle L|)\mathcal{T}^{-1}\mathcal{P}^{-1} = \rho^*\langle R| + \sigma^*\langle L| \quad ,$$

where  $\rho$  and  $\sigma$  are complex constants.

The dyadic operators  $\Omega_{ij} \equiv |i\rangle\langle j|$ , ( $i, j = R, L$ ) are thus unchanged under  $\mathcal{PT}$  transformations. Since  $\mathcal{PT}$  is antilinear, the  $\mathcal{PT}$ -transformed Hamiltonian reads

$$\begin{aligned} H_{\mathcal{PT}} &= \mathcal{PT}H\mathcal{T}^{-1}\mathcal{P}^{-1} \\ &= H_{RR}^*\Omega_{RR} + H_{RL}^*\Omega_{RL} + H_{LR}^*\Omega_{LR} + H_{LL}^*\Omega_{LL} \quad . \end{aligned} \quad (56)$$

#### 3.5.1 $H_{\mathcal{PT}} = H$

According to Eq. (56), invariance of the Hamiltonian under  $\mathcal{PT}$  leads to the equality

$$H = \begin{pmatrix} H_{RR} & H_{RL} \\ H_{LR} & H_{LL} \end{pmatrix} = \begin{pmatrix} H_{RR}^* & H_{RL}^* \\ H_{LR}^* & H_{LL}^* \end{pmatrix} = H_{\mathcal{PT}} \quad , \quad (57)$$

which shows that the matrix elements have to be real.

From the Schrödinger equation (4) and the definition of the  $L - R$  basis, it is immediate to check that, for a local potential,  $V(x)$ ,

$$H_{RR} = H_{RR}^0 + V_{RR} = k^2 + \int_{-\infty}^{+\infty} V(x)dx = H_{LL}^0 + V_{LL} = H_{LL}. \quad (58)$$

In order for  $H_{RR} = H_{LL}$  to be real, it is necessary and sufficient that the imaginary part of the integral on the *r. h. s.* of Eq. (58) vanishes, *i. e.* the imaginary part of potential  $V$  is an odd function of  $x$ . As a consequence of the reality of the off-diagonal matrix elements of  $H$ , *i. e.* of potential  $V$ , one readily obtains

$$\begin{aligned} \int_{-\infty}^{+\infty} V_r(x)\sin(2kx)dx &= 0 \\ \int_{-\infty}^{+\infty} V_i(x)\cos(2kx)dx &= 0. \end{aligned}$$

The second relation is automatically fulfilled, since  $V_i(x)$  is an odd function of  $x$ , while the first relation forces  $V_r(x)$  to be an even function.

It is easy to find how the transition operator defined in eq.(31) is affected by  $\mathcal{PT}$  invariance (reality) of the Hamiltonian,  $H$ . Indeed

$$\begin{aligned} T(t-t_0) &= \sum_{n=0}^{\infty} (-i)^n H^n (t-t_0)^n / n! \\ &= \left( \sum_{n=0}^{\infty} (i)^n H^n (t-t_0)^n / n! \right)^* \\ &= (T^{-1}(t-t_0))^* , \end{aligned}$$

and, since

$$\tilde{T}^{-1}(t-t_0) = e^{iH_0 t_0} T^{-1}(t-t_0) e^{-iH_0 t} , \quad (59)$$

$$\tilde{T}^*(t-t_0) = e^{-iH_0 t} T^*(t-t_0) e^{iH_0 t_0} , \quad (60)$$

the equality  $T^{-1}(t-t_0) = T^*(t-t_0)$  implies that

$$\lim_{t \rightarrow +\infty, t_0 \rightarrow -\infty} \tilde{T}^{-1}(t-t_0) = \lim_{t \rightarrow +\infty, t_0 \rightarrow -\infty} \tilde{T}^*(t-t_0) ,$$

hence

$$S^{-1} = S^* . \quad (61)$$

This yields for the  $S$  -matrix elements

$$\begin{aligned} S_{RL} + S_{RL}^* \det S &= 0 , \\ S_{LR} + S_{LR}^* \det S &= 0 , \\ S_{LL} &= S_{RR}^* \det S , \\ S_{RR} &= S_{LL}^* \det S . \end{aligned} \quad (62)$$

This imposes that  $S_{RL} S_{LR}^* = R_{R \rightarrow L} R_{L \rightarrow R}^*$  is real, and that

$$| \det S | = 1 \quad \text{and} \quad | S_{LL} | = | S_{RR} | , \quad (63)$$

where the latter condition corresponds to

$$| T_{L \rightarrow R} | = | T_{R \rightarrow L} | . \quad (64)$$

### 3.5.2 $H_{\mathcal{PT}} = H$ and $H_{\mathcal{T}} = H^\dagger$

Remembering that the time reversed Hamiltonian  $H_{\mathcal{T}}$  is, by definition, such that

$$\mathcal{T} H_{\mathcal{T}} = H \mathcal{T} \quad \text{and} \quad H_{\mathcal{T}} \mathcal{T} = \mathcal{T} H$$

and assuming, in addition, condition (48), certainly valid for a local potential and repeated here for clarity's sake,  $\mathcal{T} H = H^\dagger \mathcal{T}$ , forces the diagonal elements



of the Hamiltonian matrix to be equal,  $H_{LL} = H_{RR}$  ; we then see that for a  $\mathcal{PT}$ -invariant Hamiltonian the following relations hold

$$\mathcal{P}H^\dagger = H\mathcal{P} \quad \text{or} \quad H^\dagger\mathcal{P} = \mathcal{P}H$$

On the conditions given above,

$$\mathcal{P}H\mathcal{P}^{-1} = H^\dagger,$$

*i.e.*,  $H$  is pseudo-hermitian [14] with respect to  $\mathcal{P}$ .

As a consequence, the transition operator behaves as follows

$$\begin{aligned} \mathcal{P}T^\dagger(t - t_0) &= \sum_{n=0}^{\infty} (i)^n \mathcal{P}H^{\dagger n} (t - t_0)^n / n! \\ &= \sum_{n=0}^{\infty} (i)^n H^n (t - t_0)^n \mathcal{P} / n! \\ &= T^{-1}(t - t_0) \mathcal{P}. \end{aligned}$$

Hence, recalling Eq. (29),

$$\mathcal{P}\tilde{T}^\dagger(t - t_0) = \mathcal{P}e^{iH_0 t_0} e^{iH^\dagger(t-t_0)} e^{-iH_0 t} \quad (65)$$

$$= \mathcal{P}e^{iH_0 t_0} e^{i\mathcal{P}H\mathcal{P}^{-1}(t-t_0)} e^{-iH_0 t} \quad (66)$$

$$= \mathcal{P}^2 e^{iH_0 t_0} e^{iH(t-t_0)} e^{-iH_0 t} \mathcal{P}^{-1} \quad (67)$$

$$= e^{iH_0 t_0} e^{iH(t-t_0)} e^{-iH_0 t} \mathcal{P} \quad (68)$$

$$= \tilde{T}^{-1}(t - t_0) \mathcal{P} \quad (69)$$

and, in the  $t_0 \rightarrow -\infty$ ,  $t \rightarrow +\infty$  limits,

$$\mathcal{P}S^\dagger = S^{-1}\mathcal{P} \quad (70)$$

Thus, under both  $\mathcal{PT}$ -invariance of the Hamiltonian and the condition that  $H_{\mathcal{T}} = H^\dagger$ , so that the diagonal matrix elements of the Hamiltonian are real and equal,  $H_{LL} = H_{RR}$ , we have, since  $S^{-1} = S^*$ ,

$$\mathcal{P}S^\dagger = S^*\mathcal{P} \quad \text{or} \quad S^t\mathcal{P} = \mathcal{P}S. \quad (71)$$

In turn, this leads to the equality of the diagonal elements of the S matrix

$$S_{RR} = S_{LL} \implies T_{L \rightarrow R} = T_{R \rightarrow L}. \quad (72)$$

Thus

$$\begin{aligned} S_{RL} + S_{RL}^* \det S &= 0 \\ S_{LR} + S_{LR}^* \det S &= 0 \\ S_{LL} &= S_{RR} = S_{LL}^* \det S = S_{RR}^* \det S, \end{aligned}$$

which leads to

$$\det S = \frac{S_{RR}}{S_{RR}^*} = \frac{S_{LL}}{S_{LL}^*} = -\frac{S_{RL}}{S_{RL}^*} = -\frac{S_{LR}}{S_{LR}^*},$$

or, in terms of transmission and reflection coefficients,

$$\begin{aligned} |\det S| &= |T_{L \rightarrow R}/T_{L \rightarrow R}^*| = 1, \\ S_{LR}S_{RL}^* &= S_{RL}S_{LR}^* \rightarrow R_{L \rightarrow R}R_{R \rightarrow L}^* = R_{R \rightarrow L}R_{L \rightarrow R}^*, \\ R_{L \rightarrow R} + R_{L \rightarrow R}^*T_{L \rightarrow R}/T_{L \rightarrow R}^* &= 0, \\ R_{R \rightarrow L} + R_{R \rightarrow L}^*T_{R \rightarrow L}/T_{R \rightarrow L}^* &= 0. \end{aligned}$$

It is worthwhile to stress again that the equality (72) of the two transmission coefficients is not a consequence of  $\mathcal{PT}$  symmetry, which yields only the equality of their moduli, but of the additional intertwining condition (48), valid for any local potential. Again, this point is discussed in Ref. [6].

### 3.5.3 Exact Asymptotic $\mathcal{PT}$ Symmetry

In this sub-section, we consider Hamiltonians with exact  $\mathcal{PT}$  symmetry, *i. e.*  $\mathcal{PT}$ -invariant Hamiltonians whose eigenstates are also eigenstates of  $\mathcal{PT}$ .

It has been recently proved [15] that a Hamiltonian with exact  $\mathcal{PT}$  symmetry is unitarily equivalent to a Hamiltonian that is hermitian with respect to a suitably defined inner product.

Let us now investigate some consequences of exact  $\mathcal{PT}$  symmetry on the  $S$  matrix. To this aim, it is convenient to introduce the transformation under  $\mathcal{PT}$  of a generic wave function,  $\Psi(x)$

$$\mathcal{PT}\Psi(x) \equiv \Psi_{\mathcal{PT}}(x) = \Psi^*(-x) \quad (73)$$

and the condition of exact  $\mathcal{PT}$  symmetry

$$\Psi_{\mathcal{PT}}(x) = \Psi^*(-x) = e^{i\theta}\Psi(x), \quad (74)$$

where  $\theta$  is a real number, because  $(\mathcal{PT})^2 = 1$ .

Let us apply Eq. (74) to the asymptotic wave functions defined in section 2,

$$\Psi_{\mathcal{PT}}(\pm\infty) = \Psi^*(\mp\infty) = e^{i\theta}\Psi(\pm\infty), \quad (75)$$

and, in terms of their amplitudes,  $A_{\pm}$ ,  $B_{\pm}$ ,  $\tilde{A}_{\pm}$  and  $\tilde{B}_{\pm}$ ,

$$A_{\pm}^*e^{ikx} + B_{\pm}^*e^{-ikx} = e^{i\theta}(A_{\mp}e^{ikx} + B_{\mp}e^{-ikx}), \quad (76)$$

$$\tilde{A}_{\pm}^*e^{ikx} + \tilde{B}_{\pm}^*e^{-ikx} = e^{i\tilde{\theta}}(\tilde{A}_{\mp}e^{ikx} + \tilde{B}_{\mp}e^{-ikx}). \quad (77)$$

Hence, in particular

$$A_+^* = e^{i\theta}A_- , \quad \tilde{B}_+^* = e^{i\tilde{\theta}}\tilde{B}_- , \quad (78)$$

and

$$B_- = e^{-i\theta} B_+^* = 0, \quad \tilde{A}_+^* = e^{i\tilde{\theta}} \tilde{A}_- = 0. \quad (79)$$

The latter equalities come from the boundary conditions for an incident progressive wave ( $B_+ = 0$ ) and an incident regressive wave ( $\tilde{A}_- = 0$ ), respectively. The  $S$  matrix elements are thus written as

$$\begin{aligned} S_{RR} = T_{L \rightarrow R} &= \frac{A_+}{A_-} = e^{-i\theta} \frac{A_-^*}{A_-} = e^{-i(\theta+2\alpha_-)}, \quad (A_- = |A_-| e^{i\alpha_-}) \\ S_{LR} = R_{L \rightarrow R} &= \frac{B_-}{A_-} = 0, \\ S_{LL} = T_{R \rightarrow L} &= \frac{\tilde{B}_-}{\tilde{B}_+} = e^{-i\tilde{\theta}} \frac{\tilde{B}_+^*}{\tilde{B}_+} = e^{-i(\tilde{\theta}+2\tilde{\alpha}_+)}, \quad (\tilde{B}_+ = |\tilde{B}_+| e^{i\tilde{\alpha}_+}) \\ S_{RL} = R_{R \rightarrow L} &= \frac{\tilde{A}_+}{\tilde{B}_+} = 0. \end{aligned} \quad (80)$$

The reflection coefficients are thus zero and the transmission coefficients have unit modulus, in keeping with the more general condition  $|\det S| = 1$ , Eq. (63), imposed by the  $\mathcal{PT}$  symmetry of the Hamiltonian. In this case, the  $S$  matrix is unitary, too, since  $S^{-1} = S^* = (S^*)^t = S^\dagger$ .

Conversely, it is not difficult to show that conditions (80) on the  $S$  matrix elements are sufficient to ensure that the corresponding asymptotic wave functions are eigenstates of  $\mathcal{PT}$ .

Examples of  $\mathcal{PT}$ -symmetric reflectionless potentials are discussed in section 5.4.

## 4 Probability Current and Density for Linear and Antilinear Transformations

In the present section, we consider the time-dependent Schrödinger equation (1) with a local potential,  $V(x)$ , and its solution,  $\psi(x, t)$ . In this case,  $\mathcal{T}$  invariance is equivalent to hermiticity and  $V$  is real.

We introduce a linear transformation,  $U_L$ , and a corresponding antilinear transformation,  $U_A$ , commuting with the kinetic energy operator,  $p^2 = -\partial^2/\partial x^2$ , and apply them to the Schrödinger equation (1) with a local potential (3):

$$\begin{aligned} \left( -\frac{\partial^2}{\partial x^2} + V_{U_L}(x) \right) \psi_{U_L}(x, t) &= i \frac{\partial}{\partial t} \psi_{U_L}(x, t); \\ \left( -\frac{\partial^2}{\partial x^2} + V_{U_A}(x) \right) \psi_{U_A}(x, t) &= -i \frac{\partial}{\partial t} \psi_{U_A}(x, t). \end{aligned}$$

where  $\Psi_U \equiv U\Psi$  and

$$V_U(x) \equiv UV(x)U^{-1},$$

or, equivalently

$$V_U(x)U = UV(x),$$

namely, if  $V$  is invariant under  $U$ , it commutes with  $U$ .

Now, we multiply the equation satisfied by  $\psi_{U_A}$  by  $\psi$  and the initial Schrödinger equation by  $\psi_{U_A}$  and subtract them side by side, obtaining:

$$-\left(\psi_{U_A} \frac{\partial^2}{\partial x^2} \psi - \psi \frac{\partial^2}{\partial x^2} \psi_{U_A}\right) + (V - V_{U_A}) \psi_{U_A} \psi = i \frac{\partial}{\partial t} (\psi_{U_A} \psi) . \quad (81)$$

Now we introduce the density of probability current:

$$j_{U_A}(x, t) \equiv -i \left( \left( \frac{\partial}{\partial x} \psi(x, t) \right) \psi_{U_A}(x, t) - \psi(x, t) \left( \frac{\partial}{\partial x} \psi_{U_A}(x, t) \right) \right) ,$$

and the density of probability:

$$\rho_{U_A}(x, t) \equiv \psi(x, t) \psi_{U_A}(x, t) .$$

Therefore, Eq. (81) can be rewritten as:

$$\frac{\partial}{\partial x} j_{U_A} + \frac{\partial}{\partial t} \rho_{U_A} = -i (V - V_{U_A}) \rho_{U_A} . \quad (82)$$

If the potential is invariant under  $U_A$  the right-hand side of Eq. (82) is zero and we obtain a continuity equation, which, for stationary waves, yields a constant current.

Analogously, for a linear transformation, we first have to consider the complex conjugate of the equation satisfied by  $\psi_{U_L}$  and repeat the same steps as before, by replacing everywhere  $\psi_{U_A}$  by  $\psi_{U_L}^*$  and  $V_{U_A}$  by  $V_{U_L}^*$  :

$$\frac{\partial}{\partial x} j_{U_L} + \frac{\partial}{\partial t} \rho_{U_L} = -i (V - V_{U_L}^*) \rho_{U_L} . \quad (83)$$

For real  $V$ , similar considerations are valid and Eq. (83) is reduced to a continuity equation.

The formalism outlined above does not apply to non-local potentials. An attempt to extend flux conservation to the latter case is described in Ref.[16].

## 4.1 The $\mathcal{PT}$ -Symmetric Case

In the case of  $\mathcal{PT}$ -symmetric potentials, the definitions of  $\rho$  and  $j$  satisfying a continuity equation are easily obtained by writing the time-dependent Schrödinger equations satisfied by  $\psi_{\mathcal{P}}(x, t)$  and  $\psi_{\mathcal{T}}(x, t)$ :

$$\begin{aligned} \left( -\frac{\partial^2}{\partial x^2} + V(-x) \right) \psi_{\mathcal{P}}(x, t) &= i \frac{\partial}{\partial t} \psi_{\mathcal{P}}(x, t) , \\ \left( -\frac{\partial^2}{\partial x^2} + V^*(x) \right) \psi_{\mathcal{T}}(x, t) &= -i \frac{\partial}{\partial t} \psi_{\mathcal{T}}(x, t) , \end{aligned}$$

where  $\psi_{\mathcal{P}}(x, t) = \psi(-x, t)$  and  $\psi_{\mathcal{T}}(x, t) = \psi^*(x, t)$ , so that the equations given above are equivalent to the following

$$\left(-\frac{\partial^2}{\partial x^2} + V(-x)\right) \psi(-x, t) = i \frac{\partial}{\partial t} \psi(-x, t) , \quad (84)$$

$$\left(-\frac{\partial^2}{\partial x^2} + V^*(x)\right) \psi^*(x, t) = -i \frac{\partial}{\partial t} \psi^*(x, t) . \quad (85)$$

By multiplying side by side the first equation by  $\psi^*(x, t)$  and the second equation by  $\psi(-x, t)$ , and subtracting the two equations side by side, we obtain

$$\begin{aligned} & -\psi^*(x, t) \frac{\partial^2}{\partial x^2} \psi(-x, t) + \psi(-x, t) \frac{\partial^2}{\partial x^2} \psi^*(x, t) + (V(-x) - V^*(x)) \psi^*(x, t) \psi(-x, t) \\ &= i \psi^*(x, t) \frac{\partial}{\partial t} \psi(-x, t) + i \psi(-x, t) \frac{\partial}{\partial t} \psi^*(x, t) . \end{aligned}$$

$\mathcal{PT}$  invariance implies that  $V(-x) = V^*(x)$ , so that the equation above can be reduced to a continuity equation

$$\frac{\partial}{\partial x} j(x, t) + \frac{\partial}{\partial t} \rho(x, t) = 0 ,$$

with

$$\rho(x, t) = \psi^*(x, t) \psi(-x, t) , \quad (86)$$

$$j(x, t) = \frac{1}{i} [\psi^*(x, t) \frac{\partial}{\partial x} \psi(-x, t) - \psi(-x, t) \frac{\partial}{\partial x} \psi^*(x, t)] , \quad (87)$$

which is consistent with the definition of  $j$  given in Ref. [17]. The following relation holds:

$$j^*(-x, t) = -j(x, t) .$$

It is worthwhile to point out that  $j$  is identically zero when  $\psi^*(x) = e^{i\alpha} \psi(-x)$ , where  $\alpha$  is a real constant, i. e.  $\psi$  is an eigenstate of  $\mathcal{PT}$ . If  $\psi$  is a stationary wave,  $\psi(x, t) = e^{-iEt} \psi(x)$ ,  $j$  depends only on  $x$  and current (87) is constant in the whole space. The asymptotic solutions can be taken in the form of stationary waves and we obtain, remembering that, for a wave travelling from left to right, Eq.(9), we have  $B_+ = 0$ :

$$\begin{aligned} j(+\infty) &= \frac{1}{i} \left\{ \begin{aligned} & A_+^* e^{-ikx} (-ik) [A_- e^{-ikx} - B_- e^{+ikx}] \\ & - [A_- e^{-ikx} + B_- e^{+ikx}] (-ik) A_+^* e^{-ikx} \end{aligned} \right\} \\ &= 2k A_+^* B_- , \end{aligned}$$

and, in the same way

$$j(-\infty) = -2k A_+ B_-^* .$$

As expected,  $j(-\infty) = -j^*(+\infty)$ . Note that, for the reflectionless potentials discussed in sub-section 3.5.3,  $B_- = 0$ . In this case,  $j(-\infty) = j(+\infty) = 0$ .

Assuming now  $B_- \neq 0$ , conservation of current implies that we also have  $j(-\infty) = j(+\infty)$ ; hence, the current is purely imaginary and we can write:

$$A_+ B_-^* + A_+^* B_- = 0,$$

or, dividing both sides of the above equation by  $A_- A_-^*$  and remembering the definitions of  $T_{L \rightarrow R}$  and  $R_{L \rightarrow R}$ :

$$R_{L \rightarrow R} T_{L \rightarrow R}^* + R_{L \rightarrow R}^* T_{L \rightarrow R} = 0,$$

a result already obtained in sub-section 3.5.2, or, equivalently:

$$\frac{R_{L \rightarrow R}}{R_{L \rightarrow R}^*} + \frac{T_{L \rightarrow R}}{T_{L \rightarrow R}^*} = 0,$$

which means that the phase  $\varphi_r$  of the reflection coefficient and  $\varphi_t$  of the transmission coefficient are related by:

$$\varphi_r = \varphi_t + \frac{\pi}{2} + n\pi,$$

where  $n$  is an integer. This relation is trivially checked for square well [11], hyperbolic Scarf [3] and generalized Pöschl-Teller [4] potentials.

## 5 Explicit Relations for Some Potentials

For the sake of example, the formalism worked out in the previous sections is here applied in detail to a few  $\mathcal{PT}$ -symmetric solvable potentials. For those already considered in Ref. ([5]), having an imaginary part made of an odd combination of Dirac delta functions,  $\Im V(x) = \lambda \left( \delta \left( x + \frac{x_0}{2} \right) - \delta \left( x - \frac{x_0}{2} \right) \right)$ , it is easy to check that all the relations of subsection 3.5 are valid.

In the presentation of the examples, we make a selection dictated by solvability implemented by different methods.

### 5.1 Complex $\mathcal{PT}$ -Symmetric Square Well

Let

$$\begin{aligned} V &= 0, & x < -b, & \quad x > +b \\ V &= -V_0 + iV_1, & -b \leq x \leq 0, \\ V &= -V_0 - iV_1, & 0 \leq x \leq +b, \end{aligned} \tag{88}$$

Here,  $V_0$  and  $V_1$  are real parameters and  $V_0 \geq 0$ .

It is worthwhile to mention that discrete states in a  $\mathcal{PT}$ -symmetric square well with  $V_0 = 0$  were already studied in Ref.[18]. It was shown, in particular, that the square well possesses a real discrete spectrum on condition that the coefficient,  $V_1$ , of the imaginary part is smaller than a certain critical value. On

this condition, the eigenfunctions of  $H$  are also eigenfunctions of  $\mathcal{PT}$ , i. e. the model has an exact  $\mathcal{PT}$  symmetry. In this case, it is possible to construct a hermitian Hamiltonian unitarily equivalent to the  $\mathcal{PT}$ -symmetric square well in a Hilbert space endowed with a properly defined scalar product, as shown in full detail in Ref. [19]. The analysis has been extended to the continuum of scattering states in Ref.[20].

Introducing now

$$k^2 = E$$

and

$$\alpha_0^2 = E + V_0 - iV_1$$

$$\alpha_1^2 = E + V_0 + iV_1,$$

implying

$$\alpha_{0,1} = \alpha \exp(\mp i\varphi),$$

$$\alpha_0^* = \alpha_1, \quad \alpha_1^* = \alpha_0,$$

with

$$\begin{aligned} \alpha^2 &= \sqrt{(E + V_0)^2 + V_1^2} \\ \varphi &= \frac{1}{2} \arctan\left(\frac{V_1}{E + V_0}\right) \end{aligned}$$

The two linearly independent solutions (Eqs. (9-11)) can both be written in the general form

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x \leq -b \\ Ce^{i\alpha_0 x} + De^{-i\alpha_0 x} & -b \leq x \leq 0 \\ Ee^{i\alpha_1 x} + Fe^{-i\alpha_1 x} & 0 \leq x \leq b \\ Ge^{ikx} + He^{-ikx} & b \leq x \end{cases}$$

with suitable specification of parameters  $A, \dots, H$ .

The  $\mathcal{PT}$ -transformed wavefunction reads

$$\Psi_{\mathcal{PT}}(x) = \begin{cases} G^* e^{ikx} + H^* e^{-ikx} & x \leq -b \\ E^* e^{i\alpha_0 x} + F^* e^{-i\alpha_0 x} & -b \leq x \leq 0 \\ C^* e^{i\alpha_1 x} + D^* e^{-i\alpha_1 x} & 0 \leq x \leq b \\ A^* e^{ikx} + B^* e^{-ikx} & b \leq x \end{cases}$$

$\mathcal{PT}$ -symmetric wave functions would thus meet the conditions  $A = G^*$ ,  $B = H^*$ ,  $C = E^*$  and  $D = F^*$ . In the treatment of scattering states for  $V_0 = 0$ , Ref.[20] considers two linearly independent  $\mathcal{PT}$ -symmetric wave functions, in keeping with the double degeneracy and reality of the eigenvalues  $E = k^2$ . We stress, however, that these  $\mathcal{PT}$ -symmetric eigenfunctions are not the  $\Psi_1$  and  $\Psi_2$  functions (see Eqs. (12-13) studied in section 3.5.3.

We then have three pairs of continuity equations at  $x = -b$ ,  $x = 0$  and  $x = b$ , respectively :

$$\begin{pmatrix} e^{-ikb} & e^{ikb} \\ e^{-ikb} & -e^{ikb} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{-i\alpha_0 b} & e^{i\alpha_0 b} \\ \frac{\alpha_0}{k} e^{-i\alpha_0 b} & -\frac{\alpha_0}{k} e^{i\alpha_0 b} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix},$$

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{\alpha_1}{\alpha_0} & -\frac{\alpha_1}{\alpha_0} \end{pmatrix} \begin{pmatrix} E \\ F \end{pmatrix},$$

implying

$$|C|^2 + |D|^2 = |E|^2 + |F|^2,$$

$$\begin{pmatrix} e^{i\alpha_1 b} & e^{-i\alpha_1 b} \\ e^{i\alpha_1 b} & -e^{-i\alpha_1 b} \end{pmatrix} \begin{pmatrix} E \\ F \end{pmatrix} = \begin{pmatrix} e^{ikb} & e^{-ikb} \\ \frac{k}{\alpha_1} e^{ikb} & -\frac{k}{\alpha_1} e^{-ikb} \end{pmatrix} \begin{pmatrix} G \\ H \end{pmatrix}.$$

They allow to re-express the coefficients of the wave function at  $x = -\infty$  in terms of those at  $x = +\infty$

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{RR} & M_{RL} \\ M_{LR} & M_{LL} \end{pmatrix} \begin{pmatrix} G \\ H \end{pmatrix},$$

with

$$M_{i,j} = M_{i,j}(\alpha_0, \alpha_1, b, k) \quad (i, j = R, L)$$

The various matrix elements are given by the following expressions

$$M_{RR} = \frac{1}{8} e^{2ikb} \{f(\alpha_0, \alpha_1, b, k) + f(\alpha_0, -\alpha_1, b, k) \\ + f(-\alpha_0, \alpha_1, b, k) + f(-\alpha_0, -\alpha_1, b, k)\}$$

$$M_{LR} = \frac{1}{8} \{g(\alpha_0, \alpha_1, b, k) + g(\alpha_0, -\alpha_1, b, k) \\ + g(-\alpha_0, \alpha_1, b, k) + g(-\alpha_0, -\alpha_1, b, k)\}$$

$$M_{RL} = \frac{1}{8} \{h(\alpha_0, \alpha_1, b, k) + h(\alpha_0, -\alpha_1, b, k) \\ + h(-\alpha_0, \alpha_1, b, k) + h(-\alpha_0, -\alpha_1, b, k)\}$$

and

$$M_{LL} = \frac{1}{8} e^{-2ikb} \{m(\alpha_0, \alpha_1, b, k) + m(\alpha_0, -\alpha_1, b, k) \\ + m(-\alpha_0, \alpha_1, b, k) + m(-\alpha_0, -\alpha_1, b, k)\}$$

with

$$f(\alpha_0, \alpha_1, b, k) = (1 + \frac{\alpha_1}{\alpha_0})(1 + \frac{\alpha_0}{k})(1 + \frac{k}{\alpha_1})e^{-i(\alpha_0 + \alpha_1)b}$$



and

$$g(\alpha_0, \alpha_1, b, k) = (1 + \frac{\alpha_1}{\alpha_0})(1 - \frac{\alpha_0}{k})(1 + \frac{k}{\alpha_1})e^{-i(\alpha_0 + \alpha_1)b}$$

$$h(\alpha_0, \alpha_1, b, k) = (1 + \frac{\alpha_1}{\alpha_0})(1 + \frac{\alpha_0}{k})(1 - \frac{k}{\alpha_1})e^{-i(\alpha_0 + \alpha_1)b}$$

and

$$m(\alpha_0, \alpha_1, b, k) = (1 + \frac{\alpha_1}{\alpha_0})(1 - \frac{\alpha_0}{k})(1 - \frac{k}{\alpha_1})e^{-i(\alpha_0 + \alpha_1)b}$$

The obvious symmetries relating these auxiliary functions stem out

$$m(\alpha_0, \alpha_1, b, k) = f(-\alpha_0, -\alpha_1, -b, k)$$

$$h(\alpha_0, \alpha_1, b, k) = g(-\alpha_0, -\alpha_1, -b, k)$$

From these definitions, we see that

$$f(\alpha_0, \alpha_1, b, k) = f(\alpha_1, \alpha_0, b, k) = f(-\alpha_0, -\alpha_1, -b, -k) = f^*(\alpha_1, \alpha_0, -b, k)$$

$$\begin{aligned} h(\alpha_0, \alpha_1, b, k) &= -h(\alpha_1, \alpha_0, b, -k) = -h(-\alpha_1, -\alpha_0, -b, k) \\ &= h(-\alpha_0, -\alpha_1, -b, -k) = -h^*(\alpha_0, \alpha_1, -b, -k) \end{aligned}$$

A series of relations concerning the  $M$ -matrix elements follow from the above relations: some of which are listed below, not pretending to completeness (note that  $M_{RR}$  and  $M_{LL}$  are invariant under the exchange of  $\alpha_0$  and  $\alpha_1$ ) :

$$\begin{aligned} M_{RR}(\alpha_0, \alpha_1, b, k) &= M_{RR}(\alpha_1, \alpha_0, b, k) = M_{RR}(-\alpha_0, -\alpha_1, -b, -k) \\ &= M_{RR}^*(\alpha_0, \alpha_1, b, -k) \end{aligned}$$

and correspondingly for  $M_{LL}$  with, in addition,

$$M_{LL}(\alpha_0, \alpha_1, b, k) = M_{RR}(\alpha_0, \alpha_1, b, -k) = M_{RR}(-\alpha_0, -\alpha_1, -b, k),$$

while

$$\begin{aligned} M_{RL}(\alpha_0, \alpha_1, b, k) &= -M_{RL}(\alpha_1, \alpha_0, b, -k) = M_{RL}(-\alpha_0, -\alpha_1, -b, -k) \\ &= -M_{RL}^*(\alpha_0, \alpha_1, -b, -k) \end{aligned}$$

and correspondingly for  $M_{LR}$  with, in addition,

$$\begin{aligned} M_{LR}(\alpha_0, \alpha_1, b, k) &= M_{RL}(-\alpha_0, -\alpha_1, -b, k) = -M_{RL}(\alpha_1, \alpha_0, b, k) \\ &= -M_{RL}^*(\alpha_0, \alpha_1, -b, k) \end{aligned}$$

We can then give more explicit expressions for the diagonal matrix elements :

$$\begin{aligned} M_{RR} &= e^{2ikb} \cdot \left\{ \cos^2 \varphi \cos(2ab \cos \varphi) + \sin^2 \varphi \cosh(2ab \sin \varphi) - i \frac{k^2 - \alpha^2}{2k\alpha} \right. \\ &\quad \left. \cdot \sin \varphi \sinh(2ab \sin \varphi) - i \frac{k^2 + \alpha^2}{2k\alpha} \cos \varphi \sin(2ab \cos \varphi) \right\} \end{aligned}$$

and

$$M_{LL} = e^{-2ikb} \cdot \left\{ \cos^2 \varphi \cos(2ab \cos \varphi) + \sin^2 \varphi \cosh(2ab \sin \varphi) + i \frac{k^2 - \alpha^2}{2k\alpha} \cdot \sin \varphi \sinh(2ab \sin \varphi) + i \frac{k^2 + \alpha^2}{2k\alpha} \cos \varphi \sin(2ab \cos \varphi) \right\},$$

whereas the non diagonal matrix elements read

$$M_{RL} = i \left\{ \sin \varphi \cos \varphi [\cos(2ab \cos \varphi) - \cosh(2ab \sin \varphi)] + \frac{k^2 - \alpha^2}{2k\alpha} \cdot \cos \varphi \sin(2ab \cos \varphi) + \frac{k^2 + \alpha^2}{2k\alpha} \sin \varphi \sinh(2ab \sin \varphi) \right\}$$

and

$$M_{LR} = i \left\{ \sin \varphi \cos \varphi [\cos(2ab \cos \varphi) - \cosh(2ab \sin \varphi)] - \frac{k^2 - \alpha^2}{2k\alpha} \cdot \cos \varphi \sin(2ab \cos \varphi) - \frac{k^2 + \alpha^2}{2k\alpha} \sin \varphi \sinh(2ab \sin \varphi) \right\},$$

where we have used the modulus  $\alpha$  and the phase  $\varphi$  introduced earlier.

Transmission and reflection coefficients are easily expressed in terms of the  $M$ -matrix elements, on the basis of Eq. (18).

Assuming an incident wave coming from the left, i.e., from  $x = -\infty$ , the reflection and transmission amplitudes are obtained by assuming  $H = 0$

$$R_{L \rightarrow R} = \frac{M_{LR}}{M_{RR}}$$

and

$$T_{L \rightarrow R} = \frac{1}{M_{RR}},$$

which implies that

$$|R_{L \rightarrow R}|^2 + |T_{L \rightarrow R}|^2 = \frac{1 + |M_{LR}|^2}{|M_{RR}|^2}$$

and

$$R_{L \rightarrow R} T_{L \rightarrow R}^* + R_{L \rightarrow R}^* T_{L \rightarrow R} = 2 \operatorname{Re}(M_{LR}).$$

Correspondingly, we have for an incident wave coming from  $x = +\infty$

$$R_{R \rightarrow L} = -\frac{M_{RL}}{M_{RR}}$$

and

$$T_{R \rightarrow L} = \frac{\det M}{M_{RR}} = \frac{1}{M_{RR}},$$

which implies that

$$|R_{R \rightarrow L}|^2 + |T_{R \rightarrow L}|^2 = \frac{1 + |M_{RL}|^2}{|M_{RR}|^2}$$

and

$$R_{R \rightarrow L} T_{R \rightarrow L}^* + R_{R \rightarrow L}^* T_{R \rightarrow L} = -2 \operatorname{Re}(M_{RL}).$$

The two reflection amplitudes are related by the non-diagonal  $M$ -matrix elements

$$\frac{R_{R \rightarrow L}}{R_{L \rightarrow R}} = -\frac{M_{RL}}{M_{LR}}.$$

It is also easy to check that

$$\det M \equiv M_{RR}M_{LL} - M_{RL}M_{LR} = 1,$$

which amounts to  $T_{L \rightarrow R} = T_{R \rightarrow L}$ .

It is worthwhile to spend a few words on the behaviour of the transmission and reflection coefficients under the exchange of the flux generating part of the potential,  $V(x) = -V_0 + iV_1$ , with the flux absorbing part,  $V(x) = -V_0 - iV_1$ . In our notations, the exchange  $V_1 \leftrightarrow -V_1$  is equivalent to  $\alpha_0 \leftrightarrow \alpha_1$ . Since we have already noticed that  $M_{RR}$  is symmetric under that exchange, so is  $T_{L \rightarrow R} = 1/M_{RR}$  and, consequently,  $T_{R \rightarrow L} = T_{L \rightarrow R}$ .

The reflection coefficients have a different behaviour: from the relation

$$M_{LR}(\alpha_1, \alpha_0, b, k) = -M_{RL}(\alpha_0, \alpha_1, b, k),$$

we immediately deduce that

$$R_{R \rightarrow L}(\alpha_0, \alpha_1, b, k) = R_{L \rightarrow R}(\alpha_1, \alpha_0, b, k).$$

This behaviour of reflection coefficients of  $\mathcal{PT}$ -symmetric potentials was first noticed in Ref. [13] and discussed there in detail for the parallel case of the square barrier, as well as of the hyperbolic Scarf potential, to be treated in subsection 5.3.

## 5.2 Multiple Square Well

In order to extend the formalism of the preceding section to a multiple potential well, it is convenient to consider the change of the  $M$  matrix elements in the case the single well is not centred on the origin, but on an arbitrary point  $X_0$  on the real axis. Under the coordinate shift  $x' = x - X_0$ , the basic vectors are changed as follows

$$|R'\rangle = e^{-ikX_0} |R\rangle; \quad |L'\rangle = e^{ikX_0} |L\rangle,$$

and formula (23) holds, with a shift  $C = -X_0$ , so that the diagonal elements of the  $M$  matrix remain unchanged, while the off-diagonal ones are changed by a phase factor

$$\begin{pmatrix} M'_{RR} & M'_{RL} \\ M'_{LR} & M'_{LL} \end{pmatrix} = \begin{pmatrix} M_{RR} & e^{-2ikX_0} M_{RL} \\ e^{2ikX_0} M_{LR} & M_{LL} \end{pmatrix}.$$

We are thus ready to solve the simplest problem of multiple wells, i. e. two identical square wells of width  $2b$  separated by a zero-potential region of width  $2a$  centered on the origin. The  $M$  matrix of this problem is nothing but the product of the  $M$  matrices of the two wells, with off-diagonal elements properly changed in phase so as to take into account the shifts of the well centres with respect to the origin

$$M^{(dw)} = M^{(1)} \cdot M^{(2)} = \begin{pmatrix} M_{RR} & e^{2ik(a+b)} M_{RL} \\ e^{-2ik(a+b)} M_{LR} & M_{LL} \end{pmatrix} \begin{pmatrix} M_{RR} & e^{-2ik(a+b)} M_{RL} \\ e^{+2ik(a+b)} M_{LR} & M_{LL} \end{pmatrix}. \quad (89)$$

The  $M_{ij}$  elements are, of course, the same as in the preceding section.

In order to extend the above formalism to an arbitrary number,  $n$ , of identical square wells of width  $2b$  separated by intervals of constant length  $2a$ , it is convenient to introduce a new transfer matrix,  $T$ , connected with  $M$  as follows

$$\begin{pmatrix} T_{RR} & T_{RL} \\ T_{LR} & T_{LL} \end{pmatrix} = \begin{pmatrix} M_{RR} e^{-2ik(a+b)} & M_{RL} e^{2ika} \\ M_{LR} e^{-2ika} & M_{LL} e^{2ik(a+b)} \end{pmatrix}. \quad (90)$$

It is now easy to check that the  $M^{(i)}$  matrices of formula (89) can be written in terms of  $T$  in the following way

$$M^{(1)} = \mathcal{D}^*(-a-2b) \cdot T \cdot \mathcal{D}(a), \quad M^{(2)} = \mathcal{D}^*(a) \cdot T \cdot \mathcal{D}(a+2(a+b)),$$

where  $\mathcal{D}(x)$  is the diagonal matrix defined by formula (22). It is worth pointing out that the argument  $u_1 \equiv -a-2b$  of the first  $\mathcal{D}^*$  matrix is the coordinate of the left edge of the first well, while the argument  $v_1 \equiv u_1 + 2(a+b) = a$  of the first  $\mathcal{D}$  matrix corresponds to the left edge of the second well, obtained by summing to the left edge of the first well the spatial period  $2(a+b)$ . A similar interpretation holds for the arguments  $u_2 \equiv a$  and  $v_2 \equiv a + 2(a+b)$  of the second well.

Therefore, the  $M$  matrix of the double square well can be written in the very simple form

$$M = \mathcal{D}^*(-a-2b) \cdot T \cdot \mathcal{D}(a) \cdot \mathcal{D}^*(a) \cdot T \cdot \mathcal{D}(a+2(a+b)) = \mathcal{D}^*(-a-2b) \cdot T^2 \cdot \mathcal{D}(a+2(a+b)).$$

The generalization to an arbitrary number,  $n$ , of square wells with space period  $s \equiv 2(a+b)$  over an interval of length  $L = ns$  is trivial

$$M = \mathcal{D}^*(u_1) \cdot T^n \cdot \mathcal{D}(u_1 + ns).$$

In the  $n \rightarrow \infty$  limit, the above formula corresponds to the  $\mathcal{PT}$ -symmetric version of a model of one-dimensional crystal, and might be used in an analysis similar to that already carried out in Ref. [21] in the hermitian case.

### 5.3 The Hyperbolic Scarf Potential

As an another example of solvable potential, we consider the hyperbolic Scarf (or Scarf II) potential, whose scattering solutions were investigated in Ref. [22] in the hermitian case and in Ref.[3] in the  $\mathcal{PT}$ -symmetric case. This potential allows simple analytic solutions for the transmission and reflection coefficients, thus displaying explicitly the singularity structure in the complex  $k$  plane characteristic of a  $\mathcal{PT}$ -symmetric potential. General comments on these singularities as poles of the  $S$  matrix connected with bound states and resonances were recently made in ref. [6]. We repeat here the hermitian case of the Scarf II potential, because the solutions given in Ref. [22] contain several misprints. Following the notations of Ref. [3], the hermitian Scarf II potential is written in the form

$$V(x) = (\lambda^2 - s(s+1)) \frac{1}{\cosh^2 x} + \lambda(2s+1) \frac{\sinh x}{\cosh^2 x}, \quad (91)$$

where  $\lambda$  and  $s$  are real parameters. Two independent scattering solutions are:

$$F_1(x) = (1+iy)^{-\frac{s-i\lambda}{2}} (1-iy)^{-\frac{s+i\lambda}{2}} F\left(-s-ik, -s+ik, i\lambda-s+\frac{1}{2}; \frac{1+iy}{2}\right); \quad (92)$$

$$F_2(x) = (1+iy)^{\frac{s+1-i\lambda}{2}} (1-iy)^{-\frac{s+i\lambda}{2}} F\left(\frac{1}{2}-i\lambda-ik, \frac{1}{2}-i\lambda+ik, s+\frac{3}{2}-i\lambda; \frac{1+iy}{2}\right), \quad (93)$$

where  $y \equiv \sinh x$  and  $F(a, b, c; t)$  is the hypergeometric function. By exploiting the following asymptotic formula of the hypergeometric function [23]

$$\lim_{|t| \rightarrow \infty} F(a, b, c; t) = \Gamma(c) \left( \frac{\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} (-t)^{-a} + \frac{\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} (-t)^{-b} \right)$$

and the elementary limit  $\lim_{x \rightarrow \pm\infty} \sinh x = \pm \frac{\exp(\pm x)}{2}$ , we readily obtain the behaviour of  $F_1$  and  $F_2$  at  $x \rightarrow \pm\infty$ :

$$\lim_{x \rightarrow +\infty} F_1(x) = a_{1+} e^{ikx} + b_{1+} e^{-ikx},$$

with

$$a_{1+} = \frac{e^{-\frac{\pi}{2}(\lambda-k+is)}}{2^{s+2ik}} \frac{\Gamma(i\lambda-s+\frac{1}{2}) \Gamma(2ik)}{\Gamma(-s+ik) \Gamma(\frac{1}{2}+i\lambda+ik)}; \quad (94)$$

$$b_{1+} = \frac{e^{-\frac{\pi}{2}(\lambda+k+is)}}{2^{s-2ik}} \frac{\Gamma(i\lambda-s+\frac{1}{2}) \Gamma(-2ik)}{\Gamma(-s-ik) \Gamma(\frac{1}{2}+i\lambda-ik)}. \quad (95)$$

$$\lim_{x \rightarrow -\infty} F_1(x) = a_{1-} e^{ikx} + b_{1-} e^{-ikx},$$

with

$$a_{1-} = \frac{e^{\frac{\pi}{2}(\lambda+k+is)}}{2^{s-2ik}} \frac{\Gamma(i\lambda-s+\frac{1}{2}) \Gamma(-2ik)}{\Gamma(-s-ik) \Gamma(\frac{1}{2}+i\lambda-ik)}; \quad (96)$$

$$b_{1-} = \frac{e^{\frac{\pi}{2}(\lambda-k+is)}}{2^{s+2ik}} \frac{\Gamma(i\lambda - s + \frac{1}{2}) \Gamma(2ik)}{\Gamma(-s + ik) \Gamma(\frac{1}{2} + i\lambda + ik)}. \quad (97)$$

Therefore, the following relations hold

$$\begin{aligned} a_{1-} &= e^{\pi(\lambda+k+is)} b_{1+}; \\ b_{1-} &= e^{\pi(\lambda-k+is)} a_{1+}. \end{aligned}$$

The procedure is repeated for the second solution,  $F_2$ , with the following results:

$$\lim_{x \rightarrow +\infty} F_2(x) = a_{2+} e^{ikx} + b_{2+} e^{-ikx},$$

where

$$a_{2+} = \frac{e^{\frac{\pi}{2}(\lambda+k+i(s+1))}}{2^{2ik+i\lambda-\frac{1}{2}}} \frac{\Gamma(s + \frac{3}{2} - i\lambda) \Gamma(2ik)}{\Gamma(\frac{1}{2} - i\lambda + ik) \Gamma(s + 1 + ik)}; \quad (98)$$

$$b_{2+} = \frac{e^{\frac{\pi}{2}(\lambda-k+i(s+1))}}{2^{-2ik+i\lambda-\frac{1}{2}}} \frac{\Gamma(s + \frac{3}{2} - i\lambda) \Gamma(-2ik)}{\Gamma(\frac{1}{2} - i\lambda - ik) \Gamma(s + 1 - ik)}. \quad (99)$$

$$\lim_{x \rightarrow -\infty} F_2(x) = a_{2-} e^{ikx} + b_{2-} e^{-ikx},$$

where

$$a_{2-} = \frac{e^{-\frac{\pi}{2}(\lambda-k+i(s+1))}}{2^{-2ik+i\lambda-\frac{1}{2}}} \frac{\Gamma(s + \frac{3}{2} - i\lambda) \Gamma(-2ik)}{\Gamma(\frac{1}{2} - i\lambda - ik) \Gamma(s + 1 - ik)}; \quad (100)$$

$$b_{2-} = \frac{e^{-\frac{\pi}{2}(\lambda+k+i(s+1))}}{2^{2ik+i\lambda-\frac{1}{2}}} \frac{\Gamma(s + \frac{3}{2} - i\lambda) \Gamma(2ik)}{\Gamma(\frac{1}{2} - i\lambda + ik) \Gamma(s + 1 + ik)}. \quad (101)$$

Therefore:

$$\begin{aligned} a_{2-} &= e^{-\pi(\lambda-k+i(s+1))} b_{2+}; \\ b_{2-} &= e^{-\pi(\lambda+k+i(s+1))} a_{2+}. \end{aligned}$$

It is worthwhile to stress that the relations connecting  $a_{i-}$  with  $b_{i+}$  and  $b_{i-}$  with  $a_{i+}$  ( $i = 1, 2$ ) are valid not only for the hermitian potential (real  $s$  and  $\lambda$ ), but also for the  $\mathcal{PT}$ -symmetric potential with real  $s$  and imaginary  $\lambda = i\lambda'$ , provided the  $x$  coordinate is real.

After some manipulations of the  $\Gamma$  functions in the asymptotic amplitudes, it is not difficult to obtain the compact form of the  $T_{L \rightarrow R}$  and  $R_{L \rightarrow R}$  coefficients first derived in Ref.[22], corrected in Ref.[3] for a wrong sign, and repeated here for the sake of completeness:

$$T_{L \rightarrow R} = \frac{\Gamma(-s - ik) \Gamma(s + 1 - ik) \Gamma(\frac{1}{2} + i\lambda - ik) \Gamma(\frac{1}{2} - i\lambda - ik)}{\Gamma(-ik) \Gamma(1 - ik) (\Gamma(\frac{1}{2} - ik))^2}; \quad (102)$$

$$R_{L \rightarrow R} = T_{L \rightarrow R} \left( \frac{\cos(\pi s) \sinh(\pi \lambda)}{\cosh(\pi k)} + i \frac{\sin(\pi s) \cosh(\pi \lambda)}{\sinh(\pi k)} \right). \quad (103)$$

Formulae (102) hold also for the  $\mathcal{PT}$ -symmetric version of the potential with real  $s$  and imaginary  $\lambda = i\lambda'$ . In this case the hyperbolic functions of  $\lambda$  are changed into circular functions of  $\lambda'$ :  $\sinh(i\lambda') = i\sin(\lambda')$ ,  $\cosh(i\lambda') = \cos(\lambda')$ . Formulae (102) satisfy the unitarity condition

$$|T_{L \rightarrow R}|^2 + |R_{L \rightarrow R}|^2 = 1. \quad (104)$$

in the hermitian case (real  $\lambda$ ), while in the  $\mathcal{PT}$ -symmetric case (imaginary  $\lambda$ ) unitarity may be broken : for instance, when  $s$  is integer and  $\lambda/i$  half-integer,  $|T_{L \rightarrow R}|^2 + |R_{L \rightarrow R}|^2 \rightarrow \infty$  when  $k \rightarrow 0$ .

By using the general definitions of transmission and reflection coefficients, considered as functions of the coupling strength  $\lambda$ , together with the relations connecting  $a_{i\pm}$  and  $b_{i\pm}$  ( $i = 1, 2$ ), it is easy to check that  $T_{R \rightarrow L}(\lambda) = T_{L \rightarrow R}(\lambda)$  and  $R_{R \rightarrow L}(\lambda) = R_{L \rightarrow R}(-\lambda)$  in both the hermitian and the  $\mathcal{PT}$ -symmetric case mentioned above, as already noticed in Ref.[13].

A further transformation preserving  $\mathcal{PT}$  symmetry of the Scarf potential with real  $s$  and imaginary  $\lambda$  is the complex coordinate shift  $x \rightarrow x + i\epsilon$  ( $-\frac{\pi}{2} < \epsilon < +\frac{\pi}{2}$ , in order to avoid singularities in the potential).

The asymptotic forms of the two independent solutions  $F_1$  and  $F_2$  are easily computed by the procedure described in the previous pages:

$$\begin{aligned} \lim_{x \rightarrow +\infty} F_1(x + i\epsilon) &= \lim_{x \rightarrow +\infty} \left( i \frac{e^{x+i\epsilon}}{2} \right)^{-\frac{s-i\lambda}{2}} \left( -i \frac{e^{x+i\epsilon}}{2} \right)^{-\frac{s+i\lambda}{2}} \\ &\quad \cdot F \left( -s - ik, -s + ik, i\lambda - s + \frac{1}{2}; i \frac{e^{x+i\epsilon}}{4} \right) \\ &= a_{1+}(\epsilon) e^{ikx} + b_{1+}(\epsilon) e^{-ikx}, \end{aligned}$$

where

$$a_{1+}(\epsilon) = a_{1+} e^{-k\epsilon}; \quad (105)$$

$$b_{1+}(\epsilon) = b_{1+} e^{k\epsilon}. \quad (106)$$

Here,  $a_{1+}$  and  $b_{1+}$  on the right-hand-side of the previous equations are given by formulae (94) and (95), respectively. In the same way, one gets

$$\lim_{x \rightarrow -\infty} F_1(x + i\epsilon) = a_{1-}(\epsilon) e^{ikx} + b_{1-}(\epsilon) e^{-ikx},$$

with

$$a_{1-}(\epsilon) = a_{1-} e^{-k\epsilon}; \quad (107)$$

$$b_{1-}(\epsilon) = b_{1-} e^{k\epsilon}. \quad (108)$$

Here,  $a_{1-}$  and  $b_{1-}$  on the r.h.s. are obviously given by formulae (96) and (97), respectively.

The two limits of  $F_2(x + i\epsilon)$  are computed in the same way

$$\lim_{x \rightarrow \pm\infty} F_2(x + i\epsilon) = a_{2\pm}(\epsilon) e^{ikx} + b_{2\pm}(\epsilon) e^{-ikx},$$

with similar results:

$$a_{2+}(\epsilon) = a_{2+} e^{-k\epsilon}; \quad (109)$$

$$b_{2+}(\epsilon) = b_{2+} e^{k\epsilon}; \quad (110)$$

$$a_{2-}(\epsilon) = a_{2-} e^{-k\epsilon}; \quad (111)$$

$$b_{2-}(\epsilon) = b_{2-} e^{k\epsilon}. \quad (112)$$

It is thus immediate to check the result of Ref.[3]:

$$T_{L \rightarrow R}(\epsilon, \lambda) = T_{L \rightarrow R}(0, \lambda); \quad (113)$$

$$R_{L \rightarrow R}(\epsilon, \lambda) = R_{L \rightarrow R}(0, \lambda) e^{2k\epsilon}, \quad (114)$$

where the  $T_{L \rightarrow R}$  and  $R_{L \rightarrow R}$  coefficients on the r.h.s. of formulae (113-114) are given by (102). Unitarity is obviously broken by  $\epsilon \neq 0$ . Moreover, it is easy to check that, in the same case

$$T_{R \rightarrow L}(\epsilon, \lambda) = T_{L \rightarrow R}(\epsilon, \lambda); \quad (115)$$

$$R_{R \rightarrow L}(\epsilon, \lambda) = R_{L \rightarrow R}(\epsilon, -\lambda) e^{-4k\epsilon}. \quad (116)$$

## 5.4 Reflectionless Potentials

Hermitian reflectionless potentials are much studied in the literature[24, 25, 26]. In this section, we discuss two examples of reflectionless  $\mathcal{PT}$ -symmetric potentials. The first example is the regularized one-dimensional form of the "centrifugal" potential

$$V(x) = \frac{\alpha}{(x + i\varepsilon)^2}, \quad (117)$$

where  $\alpha$  is a real strength and  $\varepsilon$  a real constant that removes the singularity at the origin. The time-independent Schrödinger equation for the potential under investigation reads, in units  $\hbar = 2m = 1$

$$\left( -\frac{d^2}{dx^2} + \frac{\alpha}{(x + i\varepsilon)^2} \right) \Psi = k^2 \Psi, \quad (118)$$



We introduce the complex variable  $z = k(x + i\varepsilon)$  and express Eq. (118) in terms of  $z$ ,

$$z^2 \frac{d^2}{dz^2} \Psi + (z^2 - \alpha) \Psi = 0. \quad (119)$$

If we define the new function  $\Phi(z)$  such that  $\Psi(z) = z^{1/2} \Phi(z)$ , the equation fulfilled by  $\Phi$  is promptly obtained from Eq.(119) in the form

$$z^2 \frac{d^2}{dz^2} \Phi + z \frac{d}{dz} \Phi + \left( z^2 - \alpha - \frac{1}{4} \right) \Phi = 0, \quad (120)$$

*i.e.* a Bessel equation with square index  $\nu^2 = \alpha + 1/4$ .

A couple of linearly independent solutions to Eq.(120) with the appropriate asymptotic behaviour for  $\Psi$  to be a scattering solution to Eq.(119) is provided by the Hankel functions of first and second type,  $H_\nu^{(1)}(z)$  and  $H_\nu^{(2)}(z)$ , respectively, whose lowest order asymptotic expansions are [27]

$$\lim_{|z| \rightarrow \infty} H_\nu^{(1)}(z) = \left( \frac{2}{\pi z} \right)^{1/2} \exp \left[ i \left( z - \frac{\pi}{2} \nu - \frac{\pi}{4} \right) \right], \quad (121)$$

$$\lim_{|z| \rightarrow \infty} H_\nu^{(2)}(z) = \left( \frac{2}{\pi z} \right)^{1/2} \exp \left[ -i \left( z - \frac{\pi}{2} \nu - \frac{\pi}{4} \right) \right], \quad (122)$$

valid for  $\Re \nu > -1/2$ ,  $|\arg z| < \pi$ .

The corresponding asymptotic solutions to Eq.(119) thus are

$$\lim_{x \rightarrow \infty} \Psi_1(x) = \exp \left( ikx - k\varepsilon - i \frac{\pi}{2} \nu - i \frac{\pi}{4} \right), \quad (123)$$

$$\lim_{x \rightarrow \infty} \Psi_2(x) = \exp \left( -ikx + k\varepsilon + i \frac{\pi}{2} \nu + i \frac{\pi}{4} \right) \quad (124)$$

If the above asymptotic wave functions are written in the general form

$$\lim_{x \rightarrow \pm \infty} \Psi_i(x) = a_{i\pm} \exp(ikx) + b_{i\pm} \exp(-ikx), \quad (125)$$

we immediately obtain

$$a_{1+} = a_{1-} = \exp \left( -k\varepsilon - i \frac{\pi}{2} \nu - i \frac{\pi}{4} \right); \quad b_{1+} = b_{1-} = 0. \quad (126)$$

$$a_{2+} = a_{2-} = 0; \quad b_{2+} = b_{2-} = \exp \left( +k\varepsilon + i \frac{\pi}{2} \nu + i \frac{\pi}{4} \right). \quad (127)$$

Formulae (126) show that  $\mathcal{PT}$  is an exact symmetry for this potential. In fact, remembering Eqs. (78-79), we have in this case  $A_+ = a_{1+}$ ,  $A_- = a_{1-} = A_+$ , so that  $A_+/A_- = a_{1+}/a_{1-} = \exp(i\pi(\nu + 1/2))$ . In the same way, we get  $\tilde{B}_+ = b_{2+}$ ,  $\tilde{B}_- = b_{2-} = \tilde{B}_+$ , and  $\tilde{B}_+^*/\tilde{B}_- = b_{2+}^*/b_{2-} = \exp(-i\pi(\nu + 1/2))$ .

The resulting transmission and reflection coefficients for waves travelling from left to right and vice versa are promptly evaluated from their definition

$$T_{L \rightarrow R} = \frac{a_{2+}b_{1+} - a_{1+}b_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = 1 , \quad (128)$$

$$R_{L \rightarrow R} = \frac{b_{1+}b_{2-} - b_{1-}b_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = 0 , \quad (129)$$

$$T_{R \rightarrow L} = \frac{a_{2-}b_{1-} - a_{1-}b_{2-}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = 1 , \quad (130)$$

$$R_{R \rightarrow L} = \frac{a_{1+}a_{2-} - a_{1-}a_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = 0 . \quad (131)$$

The second example is the hyperbolic Scarf potential with integer coupling strengths,  $s = n$  and  $\lambda = im$ . The formulae of the preceding section read in this case

$$T_{L \rightarrow R} = T_{R \rightarrow L} = (-1)^{n+m} \frac{(n - ik) \dots (1 - ik)}{(n + ik) \dots (1 + ik)} \frac{(m - \frac{1}{2} - ik) \dots (\frac{1}{2} - ik)}{(m - \frac{1}{2} + ik) \dots (\frac{1}{2} + ik)} \quad (132)$$

$$R_{L \rightarrow R} = R_{L \rightarrow R} = 0 . \quad (133)$$

with  $|T_{L \rightarrow R}| = 1$ . Equations (132-133) are sufficient to ensure that the asymptotic wave functions are eigenstates of  $\mathcal{PT}$ .

Moreover, the potential possesses bound states, which, in the present parametrization, turn out to be eigenfunctions of  $\mathcal{PT}$ , as discussed in Refs.[28, 29].

In the Hermitian case, the hyperbolic Scarf potential is reflectionless only when  $s = n$  and  $\lambda = 0$ , corresponding to the well-known case of the Pöschl-Teller potential with integer coupling strength.

## 5.5 A Non-Local Potential

Let us go back to the general Schrödinger equation (1) for a monochromatic wave (2) of energy  $E = k^2$

$$-\frac{d^2}{dx^2}\Psi(x) + \lambda \int K(x, y)\Psi(y)dy = k^2\Psi(x) , \quad (134)$$

where the potential strength,  $\lambda$ , is a real number. It is easy to check, by calculating scalar products, that the kernel of a hermitian non-local potential satisfies the condition

$$K(x, y) = K^*(y, x) . \quad (135)$$

In the  $L - R$  basis,  $K$  is written as a  $2 \times 2$  hermitian matrix, as a consequence of the above constraint (135)

$$K \equiv \begin{pmatrix} K_{RR} & K_{RL} \\ K_{LR} & K_{LL} \end{pmatrix} = \begin{pmatrix} K_{RR}^* & K_{LR}^* \\ K_{RL}^* & K_{LL}^* \end{pmatrix} \equiv K^\dagger .$$

Parity invariance of the potential could be similarly checked to imply

$$K(x, y) = K(-x, -y) . \quad (136)$$

In the  $L - R$  basis, this corresponds to

$$K \equiv \begin{pmatrix} K_{RR} & K_{RL} \\ K_{LR} & K_{LL} \end{pmatrix} = \begin{pmatrix} K_{LL} & K_{LR} \\ K_{RL} & K_{RR} \end{pmatrix} \equiv \mathcal{P}K\mathcal{P}^{-1} \equiv K_{\mathcal{P}} , \quad (137)$$

as in Section 3.2.

The condition of time reversal invariance of  $K$  is obtained by using the definitions of Section 3.4.1 in the form

$$K_{\mathcal{T}} \equiv \mathcal{T}K\mathcal{T}^{-1} = \mathcal{P}K^*\mathcal{P} = K , \quad (138)$$

or, in matrix notation,

$$\begin{pmatrix} K_{RR} & K_{RL} \\ K_{LR} & K_{LL} \end{pmatrix} = \begin{pmatrix} K_{LL}^* & K_{LR}^* \\ K_{RL}^* & K_{RR}^* \end{pmatrix} , \quad (139)$$

which corresponds to

$$K(x, y) = K^*(x, y) . \quad (140)$$

Conditions similar to those of Section 3.5, therefore, lead us to introduce  $\mathcal{PT}$  invariance of  $K$  in the form

$$K_{\mathcal{PT}} \equiv \mathcal{PT}K\mathcal{T}^{-1}\mathcal{P}^{-1} = \begin{pmatrix} K_{RR}^* & K_{RL}^* \\ K_{LR}^* & K_{LL}^* \end{pmatrix} = \begin{pmatrix} K_{RR} & K_{RL} \\ K_{LR} & K_{LL} \end{pmatrix} = K . \quad (141)$$

This corresponds to

$$K(x, y) = K^*(-x, -y) , \quad (142)$$

in agreement with formula (3) of Ref.[9] , which corrects a misprint in the corresponding formula (113) of Ref.[6].

In order to deal with a solvable  $\mathcal{PT}$ -symmetric potential, we consider only separable kernels of the kind

$$K(x, y) = g(x)e^{i\alpha x}h(y)e^{i\beta y} , \quad (143)$$

where  $\alpha$  and  $\beta$  are real numbers, and  $g(x)$  and  $h(y)$  are real functions of their argument, suitably vanishing at  $\pm\infty$ .

For this kind of kernel, the hermiticity condition (135) implies  $\alpha = -\beta$  and  $g = h$ . Parity invariance (136) requires  $\alpha = \beta = 0$  and  $g(x) = g(-x)$ ,  $h(x) = h(-x)$ . Time reversal invariance (140) requires  $\alpha = \beta = 0$  , but does not impose conditions on  $g$  and  $h$ .

The various conditions that can be imposed on kernel (143) are summarized in Table I. Finally,  $\mathcal{PT}$  invariance (142) does not impose conditions on  $\alpha$  and  $\beta$ , but requires  $g(x) = g(-x)$ ,  $h(y) = h(-y)$ . As an important consequence,

Reality	$\alpha = \beta = 0$
Symmetry under $x \leftrightarrow y$	$\alpha = \beta, g = h$
Hermiticity	$\alpha = -\beta, g = h$
$\mathcal{P}$ Invariance	$\alpha = \beta = 0, g(x) = g(-x), h(y) = h(-y)$
$\mathcal{T}$ Invariance	$\alpha = \beta = 0$
$\mathcal{PT}$ Invariance	$g(x) = g(-x), h(y) = h(-y)$

Table 1: Possible symmetries of the separable kernel (143)

their Fourier transforms,  $\tilde{g}(q)$  and  $\tilde{h}(q')$ , are real even functions, too. In order to solve eq. (134), we resort to the Green's function method. As is known, the Green's function of the problem is a solution to Eq. (134) with the potential term replaced with a Dirac delta function

$$\frac{d^2}{dx^2}G_{\pm}(x, y) + (k^2 \pm i\varepsilon)G_{\pm}(x, y) = \delta(x - y). \quad (144)$$

Here, we introduce the infinitesimal positive number  $\varepsilon$  in order to shift upwards, or downwards in the complex momentum plane the singularities of the Fourier transform of the Green's function,  $G_{\pm}(q, q')$ , lying on the real axis.

In fact, after defining the Fourier transform,  $f(q)$ , of a generic function  $f(x)$  as

$$\tilde{f}(q) = \int_{-\infty}^{+\infty} f(x)e^{-iqx}dx \quad \leftrightarrow \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{f}(q)e^{iqx}dq,$$

and expressing  $G_{\pm}(x, y)$  and  $\delta(x - y)$  in terms of their Fourier transforms, we quickly solve eq. (144) for  $G_{\pm}$

$$\tilde{G}_{\pm}(q, q') = \frac{2\pi\delta(q + q')}{-q^2 + k^2 \pm i\varepsilon},$$

Therefore, the Green's function in coordinate space is

$$G_{\pm}(x, y) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{q^2 - k^2 \mp i\varepsilon} e^{iq(x-y)} dq = G_{\pm}(x - y). \quad (145)$$

The integral (145) is easily computed by the method of residues. In fact, the integrand in  $G_{+}(x - y)$  has two first order poles at  $q_1 = k + i\varepsilon'$  and  $q_2 = -k - i\varepsilon'$ , where  $\varepsilon' = \varepsilon/(2k)$ : the integral is thus computed along a contour made of the real  $q$  axis and of a half-circle of infinite radius in the upper half-plane for  $x - y > 0$ , on which the integrand vanishes, thus enclosing the pole at  $q = q_1$ , and in the lower half-plane for  $x - y < 0$ , enclosing the pole at  $q = q_2$ , for the same reason. Notice that the  $G_{+}$  contour integral is done in the counterclockwise direction for  $x - y > 0$ , while it is done in the clockwise direction for  $x - y < 0$ , so that the latter acquires a global sign opposite to the former. The result is

$$G_{+}(x - y) = -\frac{i}{2k} [e^{ik(x-y)}\theta(x - y) + e^{-ik(x-y)}\theta(y - x)], \quad (146)$$

where  $\theta(x)$  is the step function, equal to 1 for  $x > 0$  and 0 otherwise.

The second Green's function,  $G_-(x-y)$ , is the complex conjugate of  $G_+(x-y)$

$$G_-(x-y) = \frac{i}{2k} [e^{-ik(x-y)}\theta(x-y) + e^{ik(x-y)}\theta(y-x)] . \quad (147)$$

Now, we go back to eq. (134) with kernel (143), call  $\Psi_\pm(x)$  two linearly independent solutions, for a reason that will become clear in the next few lines, and define the following integral depending on  $\Psi_\pm$

$$I_\pm(\beta, k) = \int_{-\infty}^{+\infty} e^{i\beta y} h(y) \Psi_\pm(y) dy .$$

It is easy to show that  $I_\pm(\beta, k)$  can be written as a convolution of the Fourier transforms of  $h(y)$  and  $\Psi_\pm(y)$ .

The general solution to eq. (134) is thus implicitly written as

$$\Psi_\pm(x) = c_\pm e^{ikx} + d_\pm e^{-ikx} + \lambda I_\pm(\beta, k) \int_{-\infty}^{+\infty} G_\pm(x-y) g(y) e^{i\alpha y} dy . \quad (148)$$

Eq. (148) allows us to express  $I_\pm(\beta, k)$  in terms of the constants  $c_\pm$  and  $d_\pm$  and of Fourier transforms of known functions : in fact, by multiplying both sides by  $h(x)e^{i\beta x}$  and integrating over  $x$ , we obtain

$$I_\pm(\beta, k) = c_\pm \tilde{h}(k+\beta) + d_\pm \tilde{h}(k-\beta) + \lambda N_\pm(\alpha, \beta, k) I_\pm(\beta, k) , \quad (149)$$

where we have exploited the symmetry  $\tilde{h}(-k-\beta) = \tilde{h}(k+\beta)$  and  $N_\pm$  is defined as

$$\begin{aligned} N_\pm(\alpha, \beta, k) &= \int_{-\infty}^{+\infty} h(x) e^{i\beta x} G_\pm(x-y) g(y) e^{i\alpha y} dx dy \\ &= \mp \frac{i}{2k} \int_{-\infty}^{+\infty} h(x) e^{i\beta x} e^{\pm ik|x-y|} g(y) e^{i\alpha y} dx dy, \end{aligned} \quad (150)$$

so that

$$I_\pm(\beta, k) = \frac{c_\pm \tilde{h}(k+\beta) + d_\pm \tilde{h}(k-\beta)}{1 - \lambda N_\pm(\alpha, \beta, k)} = (c_\pm \tilde{h}(k+\beta) + d_\pm \tilde{h}(k-\beta)) D_\pm , \quad (151)$$

where

$$D_\pm(\alpha, \beta, k) \equiv \frac{1}{1 - \lambda N_\pm(\alpha, \beta, k)} .$$

Let us examine now the asymptotic behaviour of the two independent solutions, starting from  $\Psi_+(x)$

$$\Psi_+(x) = c_+ e^{ikx} + d_+ e^{-ikx} + \lambda I_+(\beta, k) \int_{-\infty}^{+\infty} G_+(x-y) g(y) e^{i\alpha y} dy . \quad (152)$$

The asymptotic behaviour of the integral on the r. h. s. of eq. (152) is promptly evaluated by observing that, according to eq. (146),

$$\lim_{x \rightarrow \pm\infty} G_+(x-y) = -\frac{i}{2k} e^{\pm ik(x-y)},$$

so that

$$\lim_{x \rightarrow \pm\infty} \Psi_+(x) = c_+ e^{ikx} + d_+ e^{-ikx} - i\omega I_+(\beta, k) \tilde{g}(k \mp \alpha) e^{\pm ikx},$$

where we have put  $\omega = \lambda/(2k)$ .

Remembering the expression (151) of  $I_+$ , we finally obtain

$$\begin{aligned} \lim_{x \rightarrow -\infty} \Psi_+(x) &= c_+ e^{ikx} + \left\{ d_+ - i\omega \tilde{g}(k + \alpha) \left[ c_+ \tilde{h}(k + \beta) + d_+ \tilde{h}(k - \beta) \right] D_+ \right\} e^{-ikx}, \\ \lim_{x \rightarrow +\infty} \Psi_+(x) &= \left\{ c_+ - i\omega \tilde{g}(k - \alpha) \left[ c_+ \tilde{h}(k + \beta) + d_+ \tilde{h}(k - \beta) \right] D_+ \right\} e^{ikx} + d_+ e^{-ikx}. \end{aligned}$$

The constants  $c_+$  and  $d_+$  are fixed by initial conditions: if we impose that  $\Psi_+(x)$  represents a wave travelling from left to right, according to formula (12), we immediately have  $c_+ = 1$ ,  $d_+ = 0$  and

$$\begin{aligned} T_{L \rightarrow R} &= 1 - i\omega \tilde{g}(k - \alpha) \tilde{h}(k + \beta) D_+(\alpha, \beta, k), \\ R_{L \rightarrow R} &= -i\omega \tilde{g}(k + \alpha) \tilde{h}(k + \beta) D_+(\alpha, \beta, k). \end{aligned} \quad (153)$$

It is worthwhile to point out that the above expressions break unitarity, i.e.  $|T_{L \rightarrow R}|^2 + |R_{L \rightarrow R}|^2 \neq 1$ , because probability flux is not conserved in general.

We come now to the second solution,  $\Psi_-(x)$ , written in the form

$$\Psi_-(x) = c_- e^{ikx} + d_- e^{-ikx} + \lambda I_-(\beta, k) \int_{-\infty}^{+\infty} G_-(x-y) g(y) e^{i\alpha y} dy. \quad (154)$$

The asymptotic behaviour of the Green's function,  $G_-(x)$ , is now

$$\lim_{x \rightarrow \pm\infty} G_-(x-y) = \frac{i}{2k} e^{\mp ik(x-y)},$$

so that

$$\lim_{x \rightarrow \pm\infty} \Psi_-(x) = c_- e^{ikx} + d_- e^{-ikx} + i\omega I_-(\beta, k) \tilde{g}(k \pm \alpha) e^{\mp ikx},$$

or, using the explicit expression (151) of  $I_-$ ,

$$\begin{aligned} \lim_{x \rightarrow -\infty} \Psi_-(x) &= d_- e^{-ikx} + \left\{ c_- + i\omega \tilde{g}(k - \alpha) \left[ c_- \tilde{h}(k + \beta) + d_- \tilde{h}(k - \beta) \right] D_- \right\} e^{ikx}, \\ \lim_{x \rightarrow +\infty} \Psi_-(x) &= c_- e^{ikx} + \left\{ d_- + i\omega \tilde{g}(k + \alpha) \left[ c_- \tilde{h}(k + \beta) + d_- \tilde{h}(k - \beta) \right] D_- \right\} e^{-ikx}. \end{aligned}$$

Since  $\Psi_-(x)$  and  $\Psi_+(x)$  are linearly independent, we can impose that  $\Psi_-(x)$  is a wave travelling from right to left, according to formula (13); the initial conditions are

$$\begin{aligned} c_- + i\omega\tilde{g}(k - \alpha)(c_- \tilde{h}(k + \beta) + d_- \tilde{h}(k - \beta))D_-(\alpha, \beta, k) &= 0, \\ d_- + i\omega\tilde{g}(k + \alpha)(c_- \tilde{h}(k + \beta) + d_- \tilde{h}(k - \beta))D_-(\alpha, \beta, k) &= 1, \end{aligned}$$

where

$$d_- = T_{R \rightarrow L}, \quad c_- = R_{R \rightarrow L}. \quad (155)$$

We then obtain

$$\begin{aligned} T_{R \rightarrow L} &= 1 - i\omega\tilde{g}(k + \alpha)\tilde{h}(k - \beta)\mathcal{D}_-(\alpha, \beta, k), \\ R_{R \rightarrow L} &= -i\omega\tilde{g}(k - \alpha)\tilde{h}(k - \beta)\mathcal{D}_-(\alpha, \beta, k). \end{aligned} \quad (156)$$

where

$$\mathcal{D}_-(\alpha, \beta, k) = \frac{1}{1 - \lambda N_- + i\omega(\tilde{g}(k + \alpha)\tilde{h}(k - \beta) + \tilde{g}(k - \alpha)\tilde{h}(k + \beta))}.$$

Formulae (154-155) show that, in general, for a  $\mathcal{PT}$ -symmetric non-local potential,  $T_{R \rightarrow L} \neq T_{L \rightarrow R}$ . In fact, from the quoted formulae,

$$T_{R \rightarrow L} - T_{L \rightarrow R} = i\omega\Delta D_+(\alpha, \beta, k)\mathcal{D}_-(\alpha, \beta, k),$$

where

$$\begin{aligned} \Delta &= \tilde{g}(k - \alpha)\tilde{h}(k + \beta) - \tilde{g}(k + \alpha)\tilde{h}(k - \beta) \\ &\quad + \lambda(N_+ \tilde{g}(k + \alpha)\tilde{h}(k - \beta) - N_- \tilde{g}(k - \alpha)\tilde{h}(k + \beta)) \\ &\quad + i\omega\tilde{g}(k - \alpha)\tilde{h}(k + \beta)(\tilde{g}(k + \alpha)\tilde{h}(k - \beta) + \tilde{g}(k - \alpha)\tilde{h}(k + \beta)). \end{aligned}$$

Computation of the  $N_{\pm}$  integrals yields the general forms

$$\begin{aligned} \lambda N_+(\alpha, \beta, k) &= -i\frac{\omega}{2} \left[ \tilde{g}(k - \alpha)\tilde{h}(k + \beta) + \tilde{g}(k + \alpha)\tilde{h}(k - \beta) \right] + Q(\alpha, \beta, k), \\ \lambda N_-(\alpha, \beta, k) &= i\frac{\omega}{2} \left[ \tilde{g}(k - \alpha)\tilde{h}(k + \beta) + \tilde{g}(k + \alpha)\tilde{h}(k - \beta) \right] + Q(\alpha, \beta, k), \end{aligned}$$

where the function  $Q(\alpha, \beta, k)$  is real.

If we now make the additional assumption that our kernel is symmetric,  $K(x, y) = K(y, x)$ , i.e.  $g = h$  and  $\alpha = \beta$ , we obtain  $T_{R \rightarrow L} = T_{L \rightarrow R}$ . It is worthwhile to stress that imposing the symmetry of the kernel is equivalent to imposing the intertwining condition (48), i.e.  $K_{\mathcal{T}} = K^{\dagger}$ , which ensures the equality of the two transmission coefficients.

A detailed calculation for the case

$$g(x) = e^{-\gamma|x|}, \quad h(y) = e^{-\delta|y|},$$

with  $\gamma$  and  $\delta$  positive numbers, i.e. the Yamaguchi potential, has been presented in Ref. [30].

Unitarity properties are discussed therein: in particular, when the Yamaguchi potential is  $\mathcal{PT}$ -symmetric with non-zero  $\alpha$  and  $\beta$ , the characteristics of unitarity breaking are distinctly different from those of  $\mathcal{PT}$ -symmetric local potentials discussed in Ref. [13].

## 6 Conclusions

In this final section, we try to focus attention on what we believe are the most original results of our investigation.

Exact  $\mathcal{PT}$  invariance has been introduced in the literature as a condition on the bound-state eigenfunctions of a  $\mathcal{PT}$ -symmetric Hamiltonian. The conclusion is the following: the eigenstates of  $H$  should be eigenstates of  $\mathcal{PT}$ , too. In turn, this condition ensures that the corresponding eigenvalues are real.

As a particular example, we mention the imaginary  $\mathcal{PT}$ -symmetric square well studied in Ref.[18]. There, a well defined threshold was found for the discrete spectrum, separating the regime of exact  $\mathcal{PT}$  symmetry from that of spontaneously broken symmetry. In the case of scattering, an extension of these results might be ambiguous, in so far as the continuum can always be labelled with a real energy,  $E = k^2$ . Correspondingly, Ref.[20] shows that one can always find  $\mathcal{PT}$ -symmetric continuum eigenfunctions of this Hamiltonian, both below and above the critical potential strength found in Ref.[18].

In our considerations, we have tried to introduce a specific "exact"  $\mathcal{PT}$  invariance associated with the scattering states of type (12) and (13). We have called this this condition exact asymptotic  $\mathcal{PT}$  symmetry, which is only and specifically relevant to scattering; we have shown that this condition forces the  $\mathcal{PT}$ -symmetric potential to be reflectionless (the above mentioned  $\mathcal{PT}$ -symmetric square well does not belong to this class).

While the interest in reflectionless potentials was recently revived in the frame of supersymmetric quantum mechanics and Darboux transformations[26], we stress the fact that the potentials considered in Ref.[26] are real. Our link of exact asymptotic  $\mathcal{PT}$  invariance with reflectionless complex  $\mathcal{PT}$ -symmetric potentials should provide the necessary stimulus to broaden the investigation[2, 10] and classification of reflectionless potentials so as to include their complex form, of which we have provided a few examples in the present work.

The other most important topic we have elaborated concerns the delicate distinction and interplay between hermiticity and time reversal invariance for non-local potentials and a proper extension of  $\mathcal{PT}$  invariance to this case.

An explicit construction of a solvable separable complex potential has been presented and worked out in detail in Ref. [30]. A particularly notable difference between local and non-local  $\mathcal{PT}$ -symmetric potentials is the non-equality of the two transmission coefficients in the non-local case; they have also a quite different behaviour in unitarity breaking [13, 30].

An extension of the present work can be envisaged for multi-channel problems[31, 32, 33], with the specific aim to formulate a self-contained and consistent framework to extend the discussion of symmetry properties to elastic scattering of non-zero spin particles and to inelastic scattering.



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